

## Supporting Information

# Diverse and chemoselective sigmatropic shift rearrangements of multisubstituted *N,O*-diarylhydroxylamines

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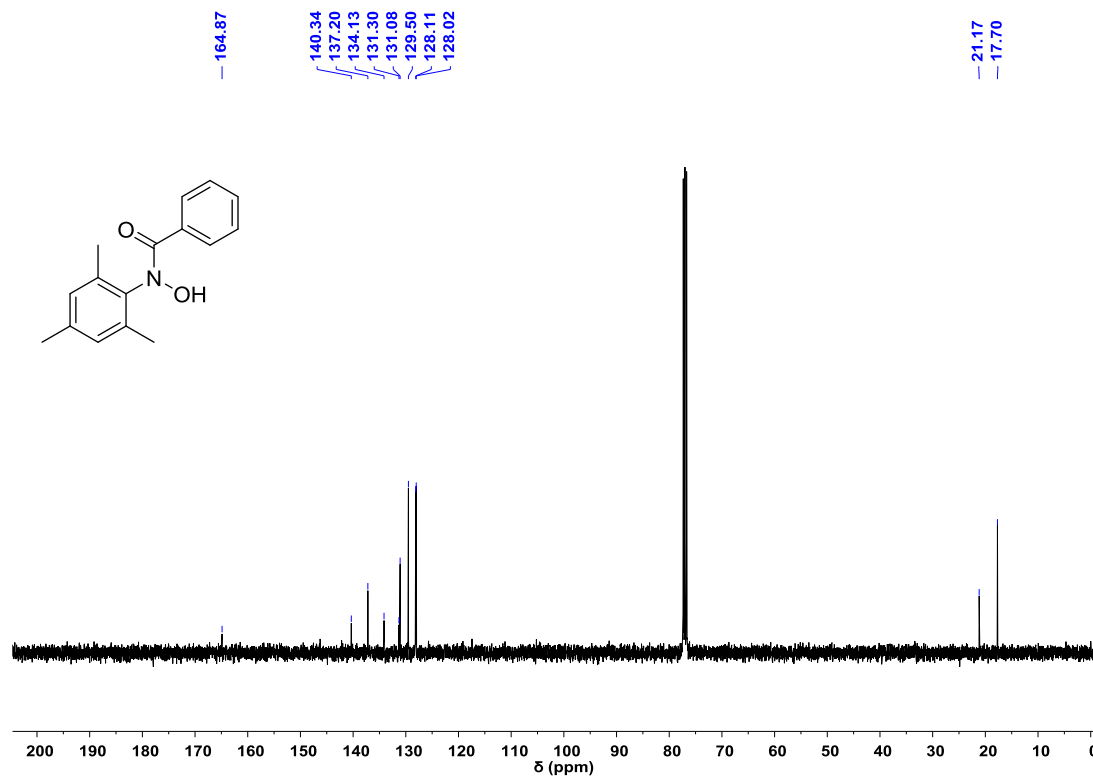
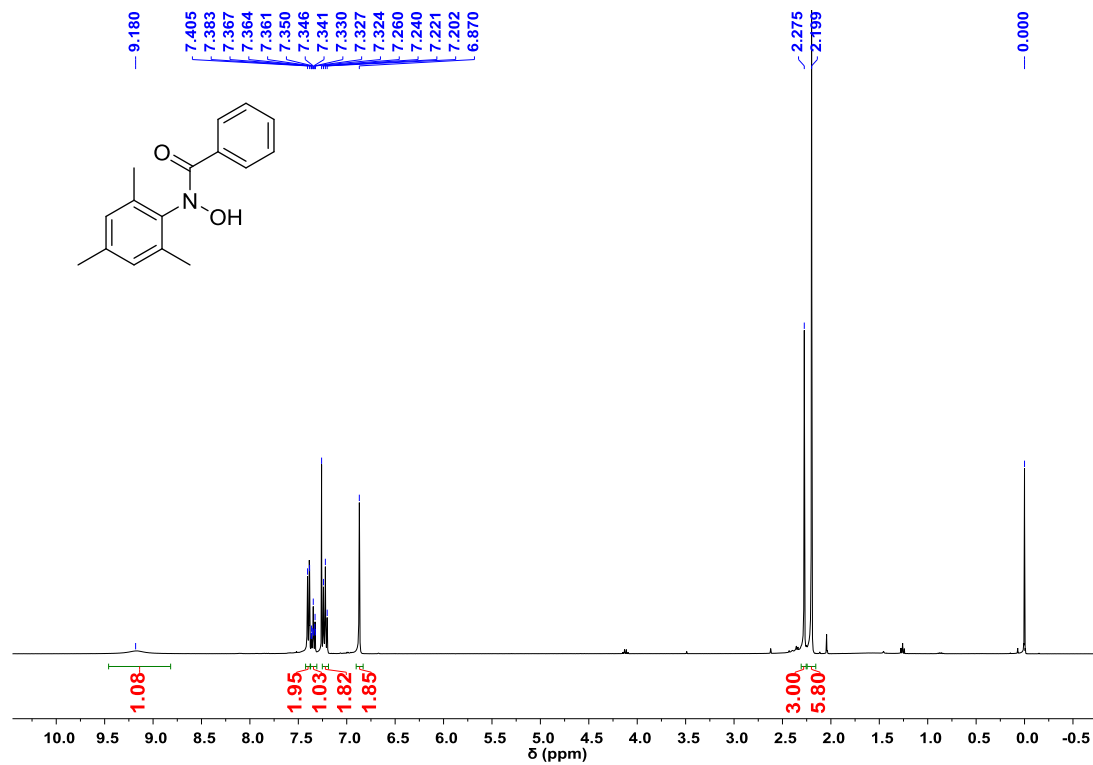
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### Copies of NMR spectra of product 1

$^1\text{H}$  NMR (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) in  $\text{CDCl}_3$

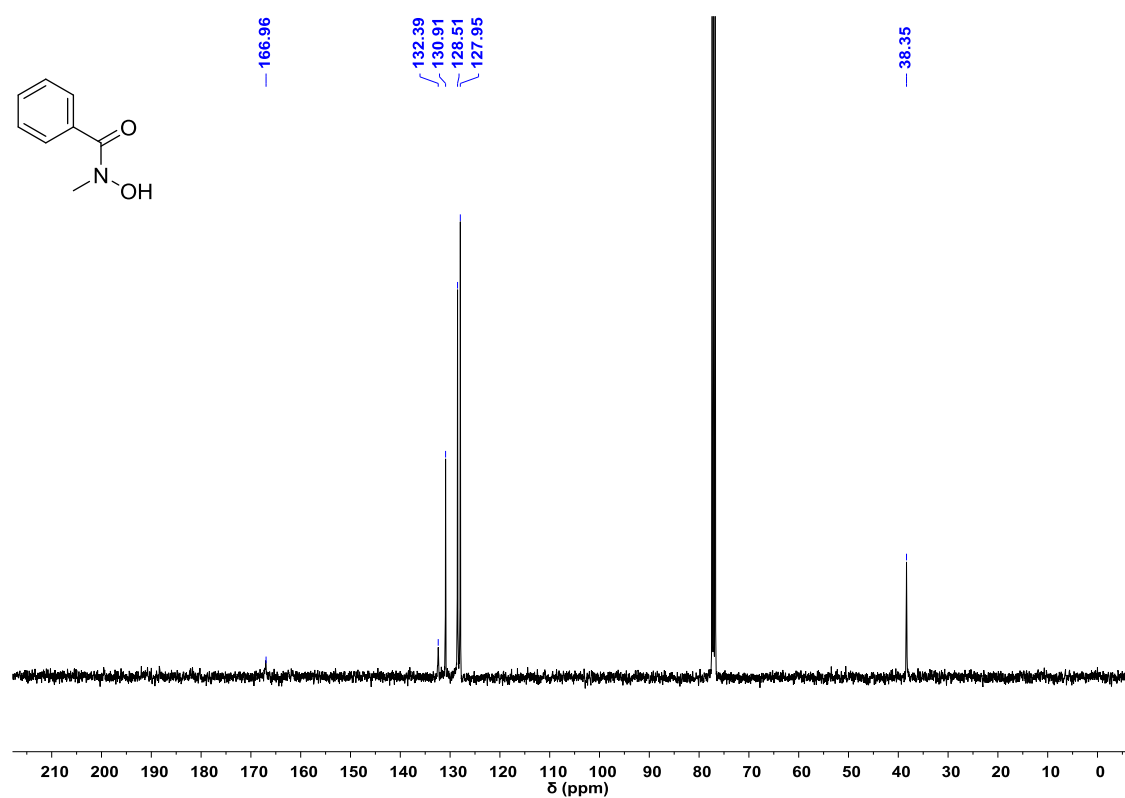
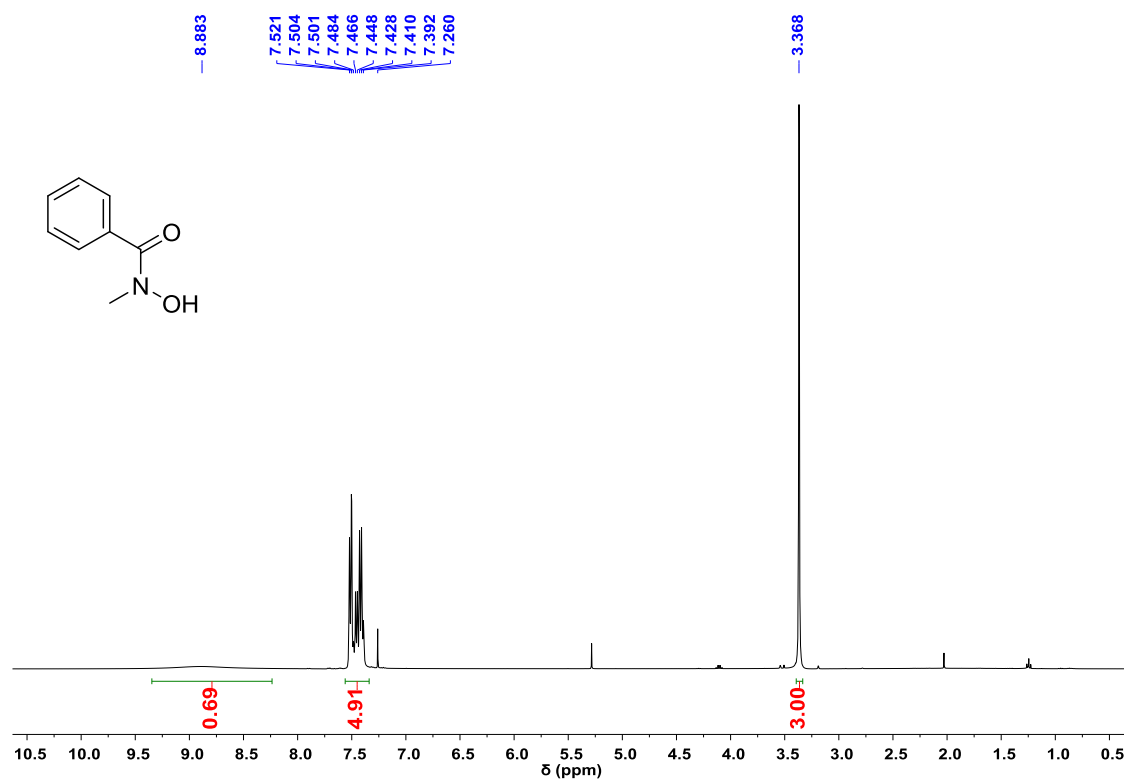
#### *N*-Hydroxy-*N*-mesitylbenzamide (**1**)



## Copies of NMR spectra of product 8

$^1\text{H}$  NMR (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) in  $\text{CDCl}_3$

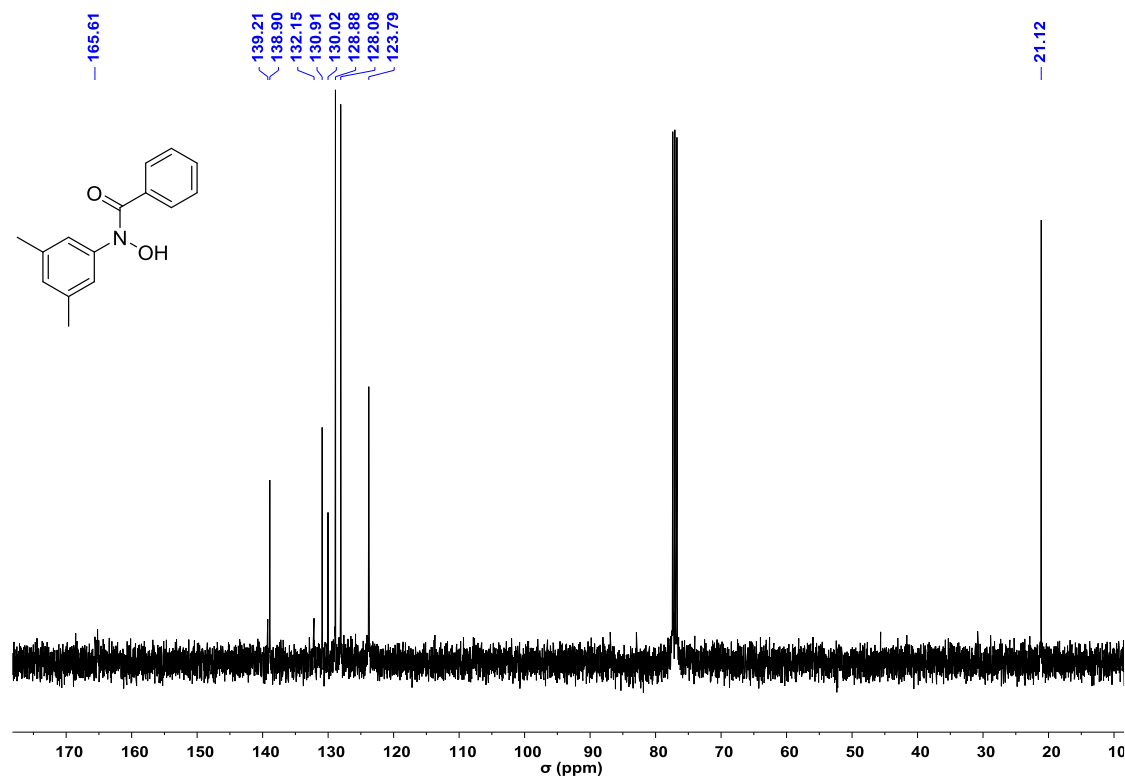
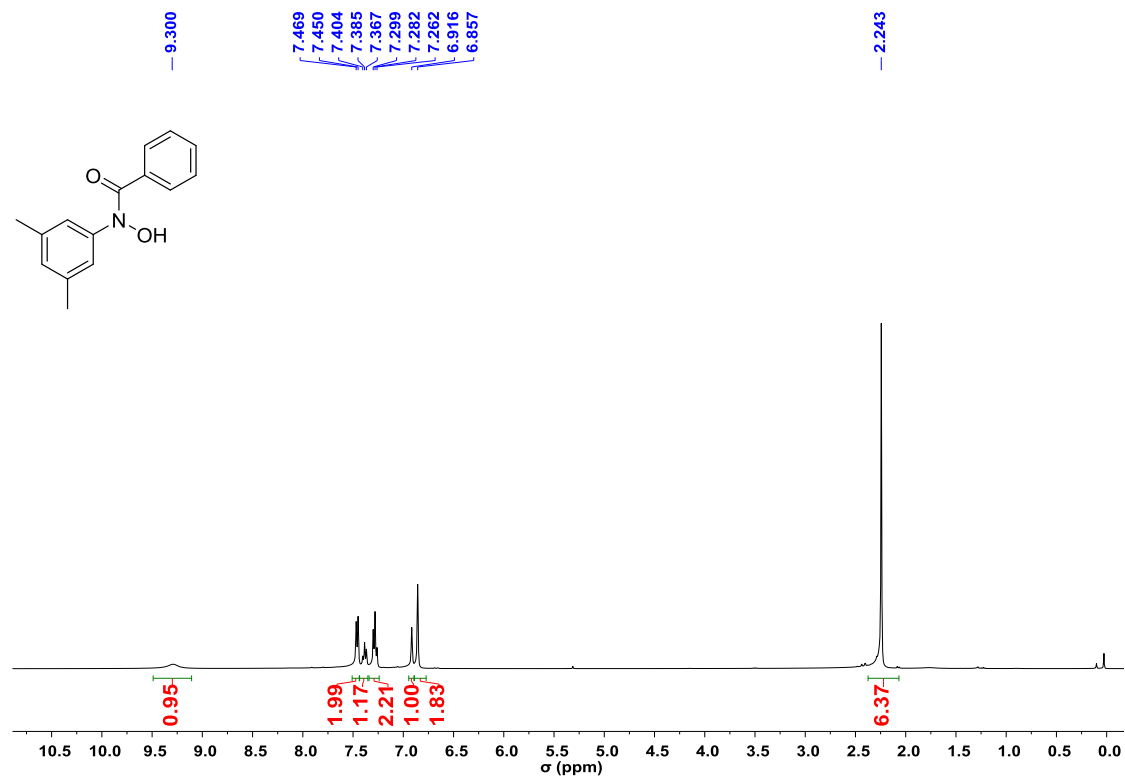
*N*-Hydroxy-*N*-methylbenzamide (**8**)



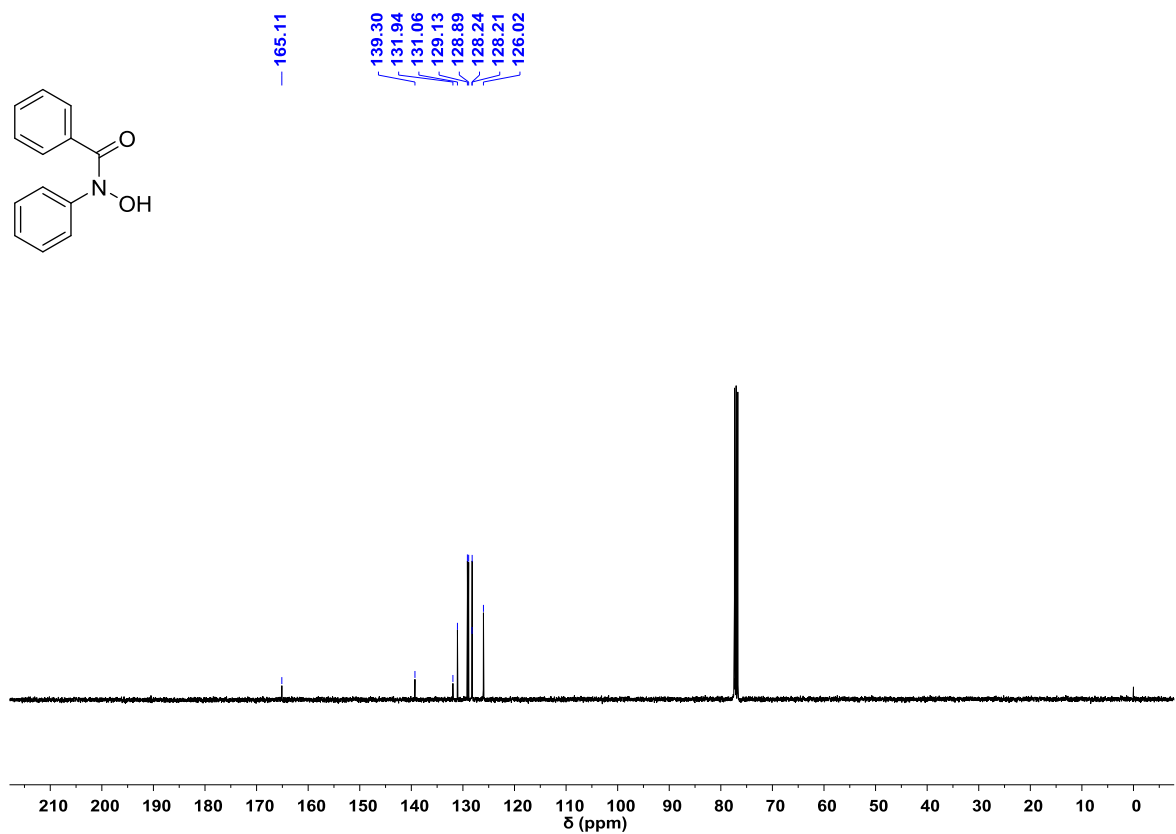
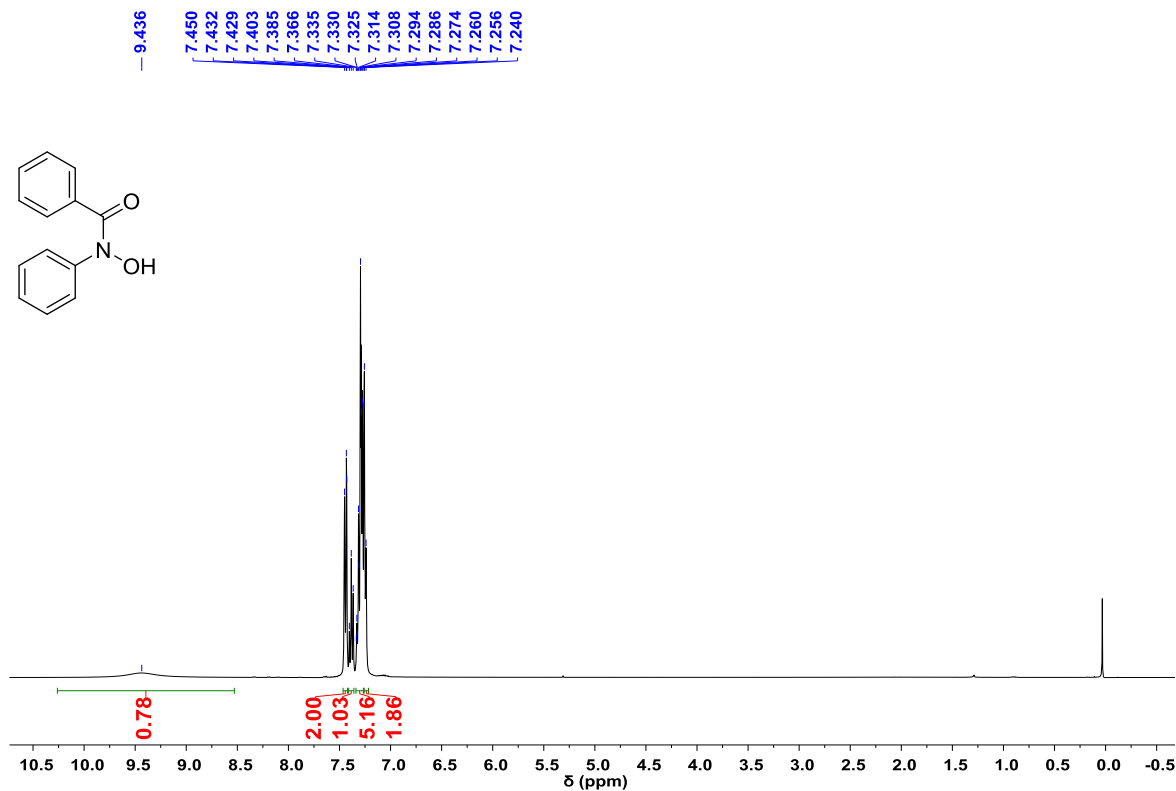
### Copies of NMR spectra of products 11

$^1\text{H}$  NMR (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) in  $\text{CDCl}_3$

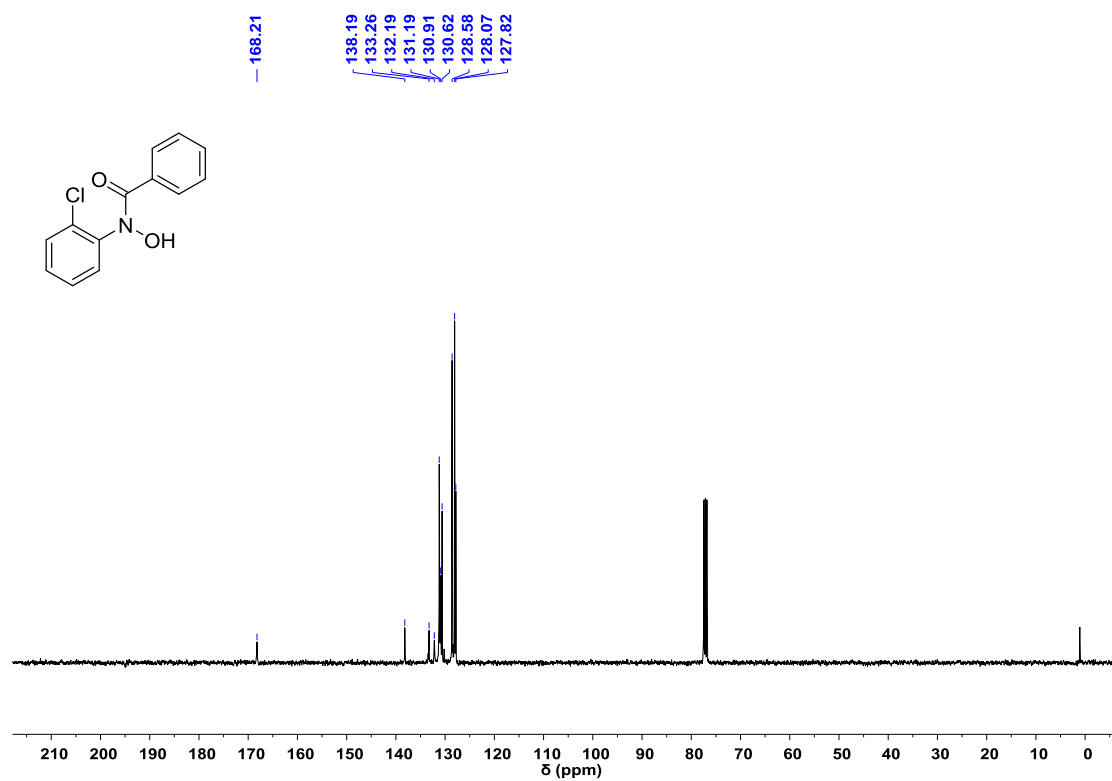
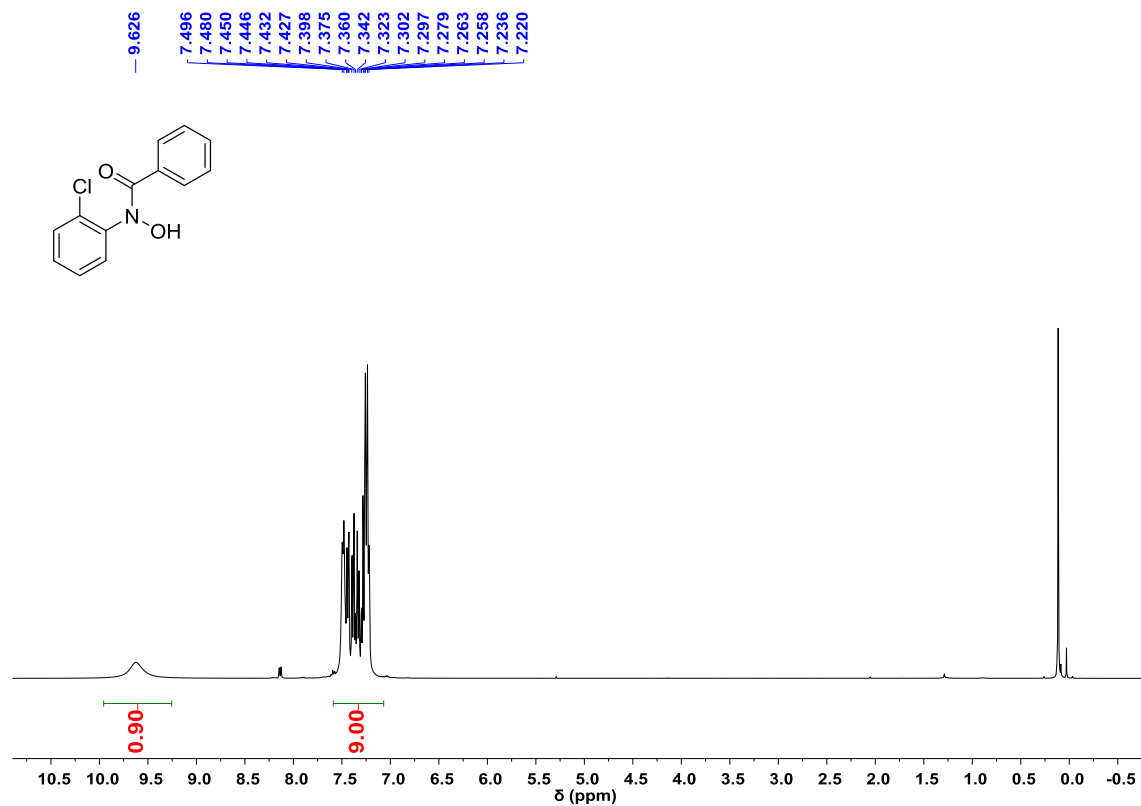
*N*-(3,5-Dimethylphenyl)-*N*-hydroxybenzamide (**11e**)



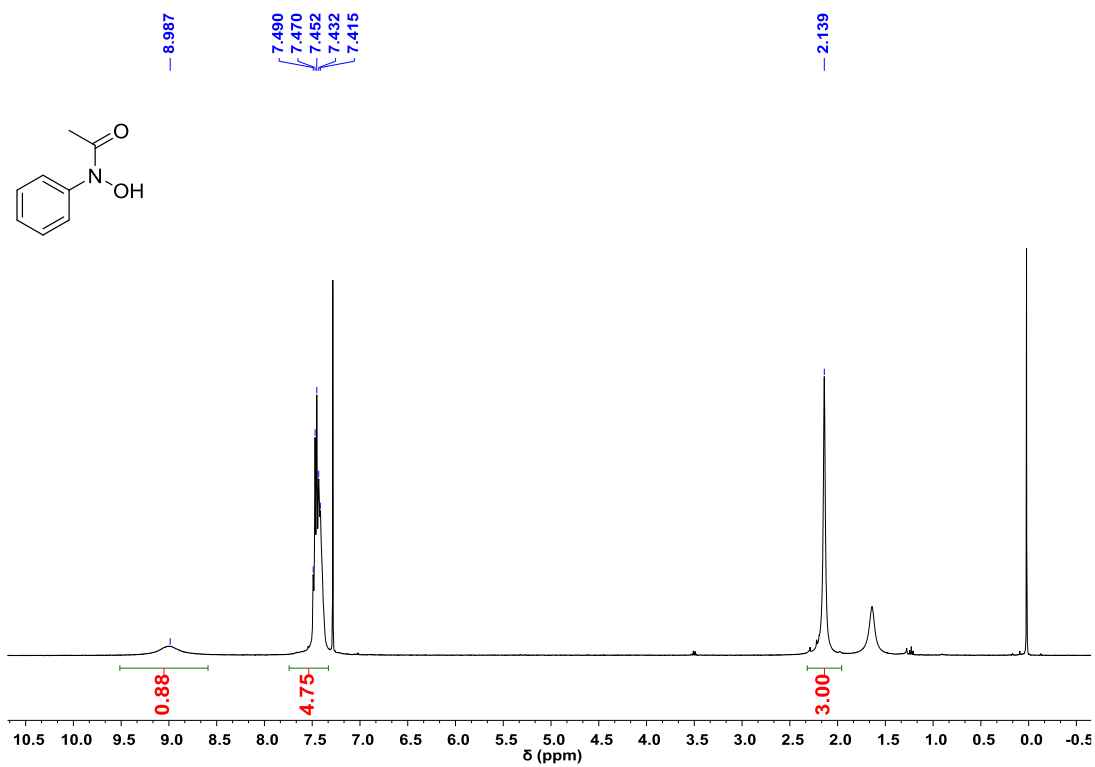
*N*-hydroxy-*N*-(*p*-tolyl)acetamide (**11g**)



### *N*-(2-Chlorophenyl)-*N*-hydroxybenzamide (**11h**)



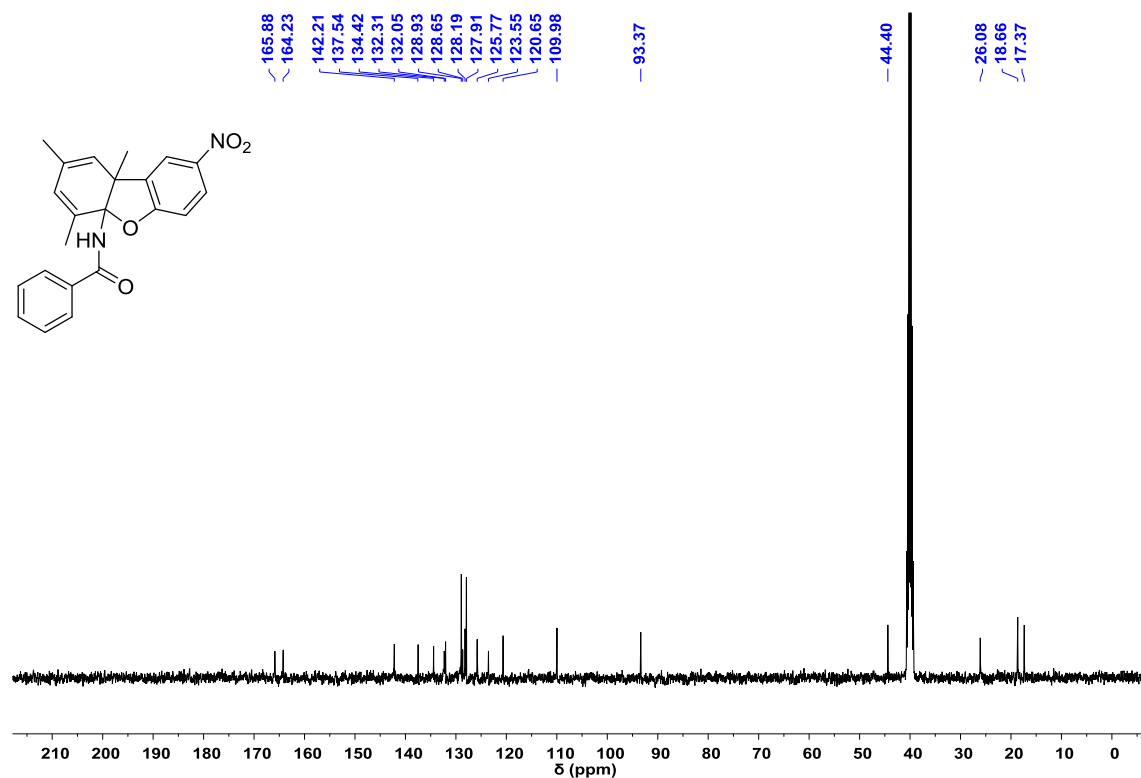
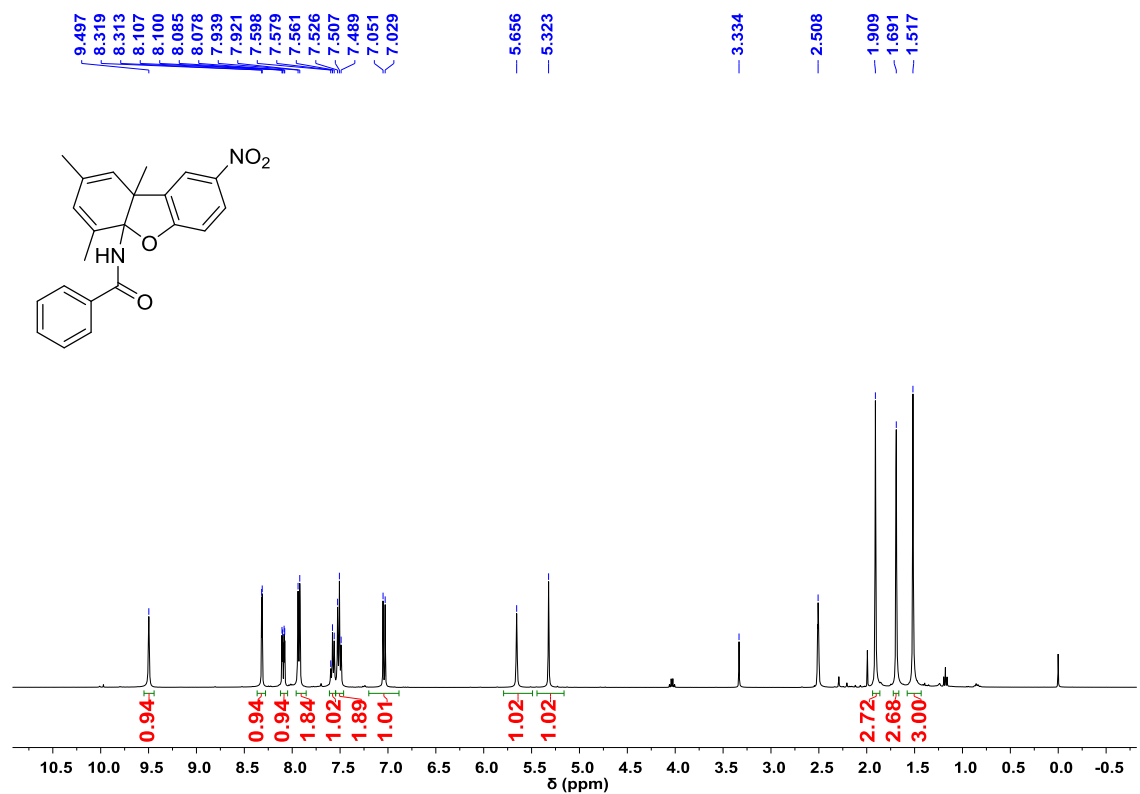
### *N*-Hydroxy-*N*-phenylacetamide (**11i**)



### Copies of NMR spectra of products 3

$^1\text{H}$  NMR (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) in  $\text{DMSO-}d_6$

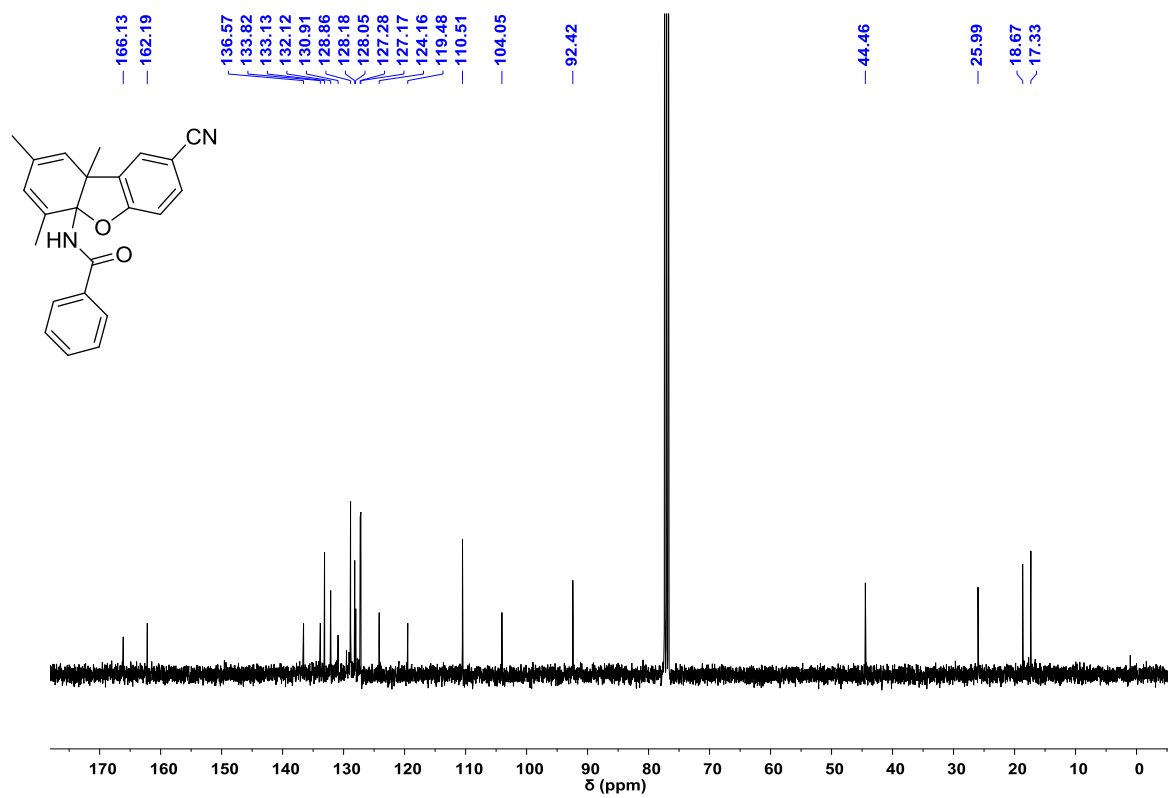
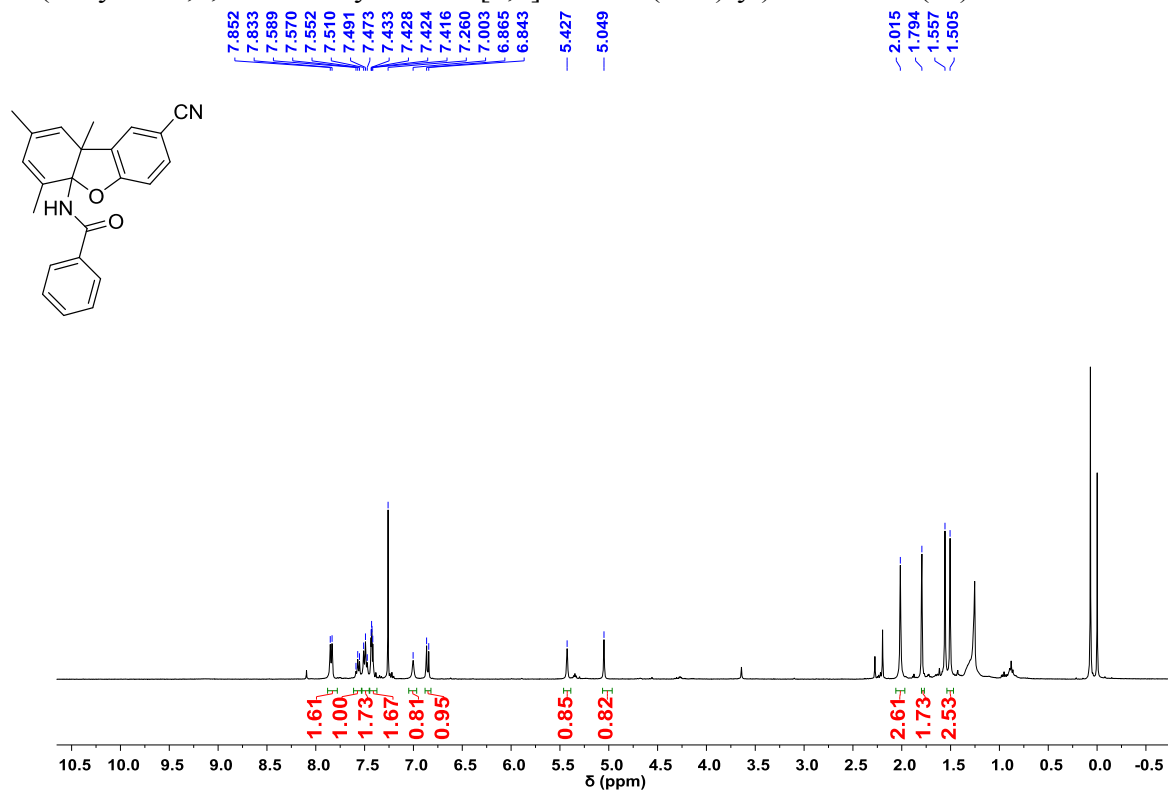
*N*-(2,4,9b-Trimethyl-8-nitrodibenzo[*b,d*]furan-4a(9*bH*)-yl)benzamide (**3a**)





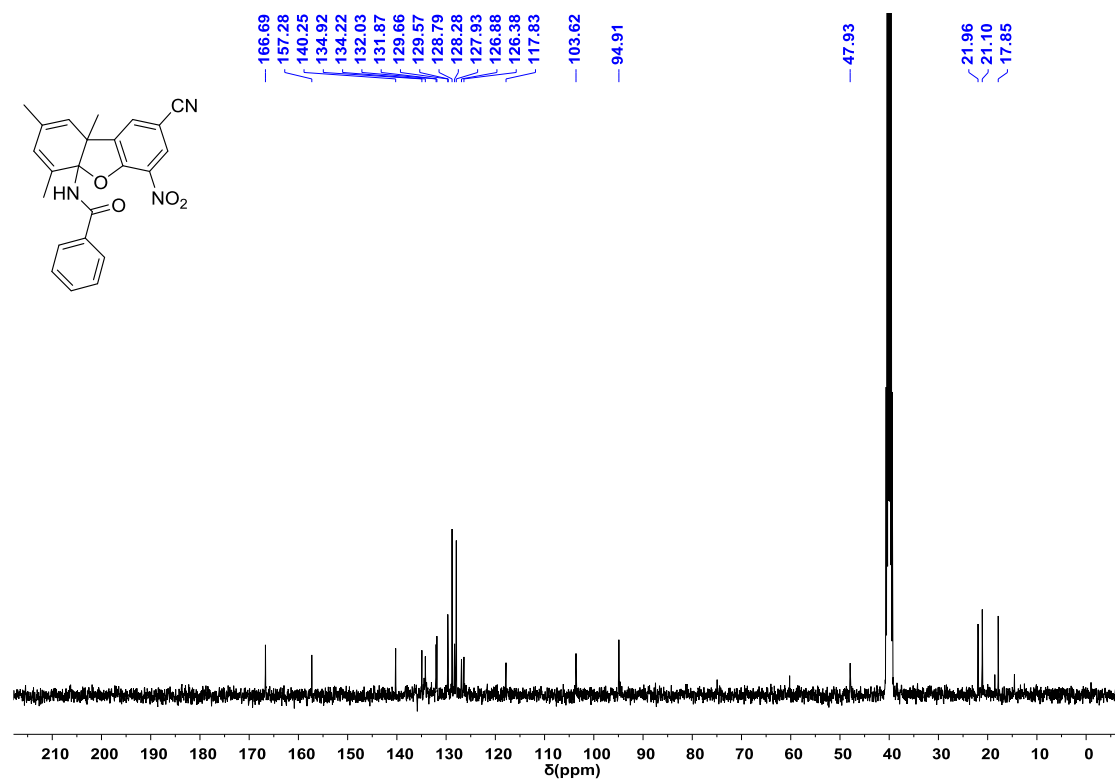
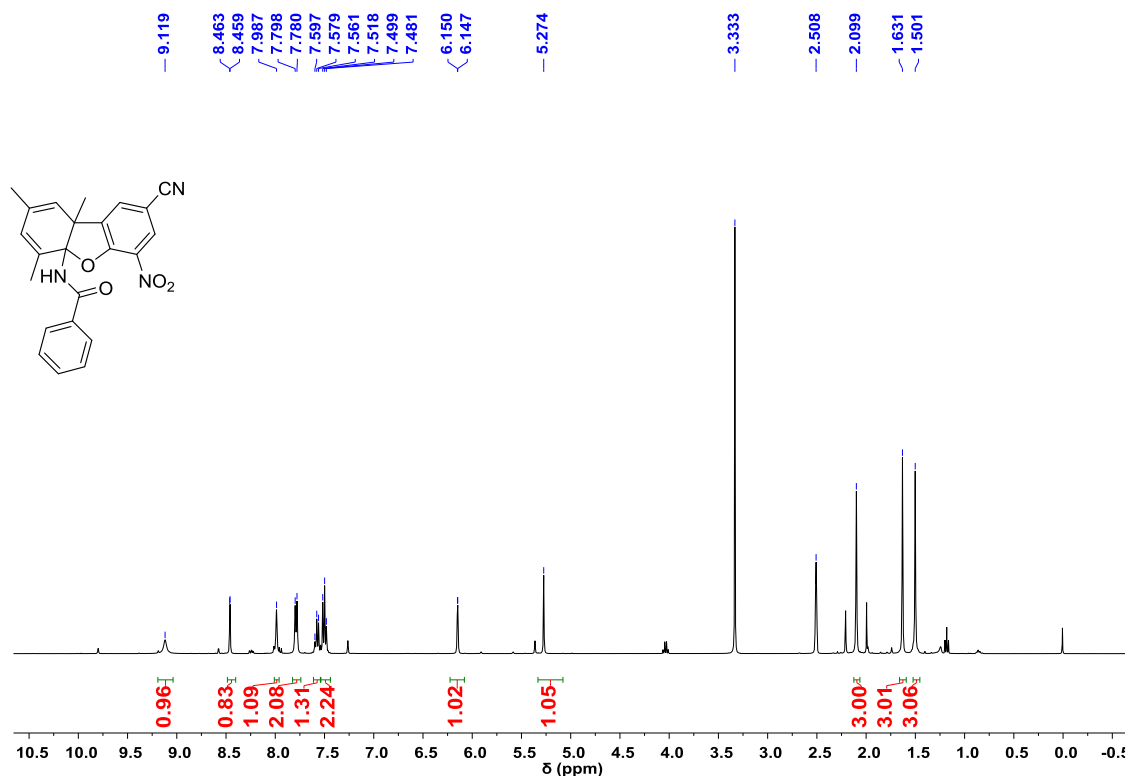
$^1\text{H}$  NMR (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) in  $\text{CDCl}_3$

*N*-(8-Cyano-2,4,9b-trimethyldibenzo[*b,d*]furan-4a(9*bH*)-yl)benzamide (**3c**)



$^1\text{H}$  NMR (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) in  $\text{DMSO-}d_6$

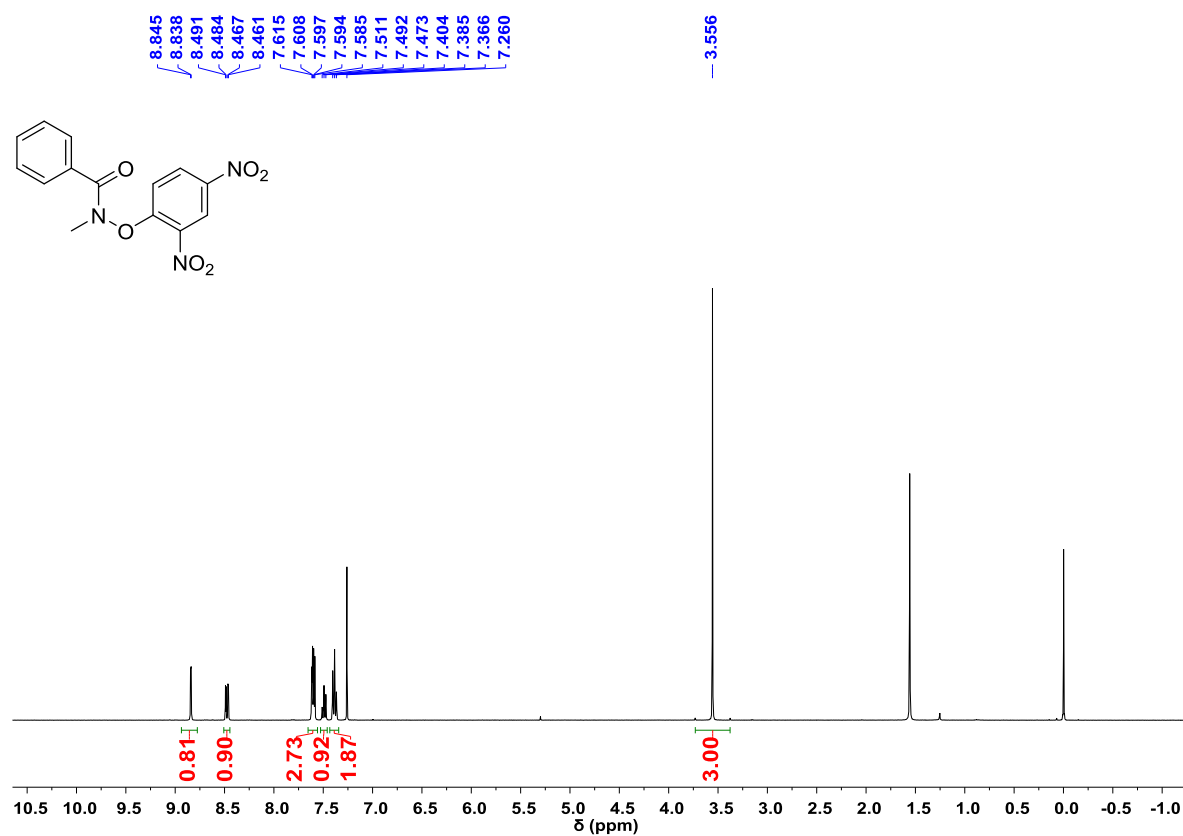
*N*-(8-Cyano-2,4,9b-trimethyl-6-nitrodibenzo[*b,d*]furan-4a(9*bH*)-yl)benzamide (**3d**)



### Copy of NMR spectra of product 9

$^1\text{H}$  NMR (400 MHz) in  $\text{CDCl}_3$

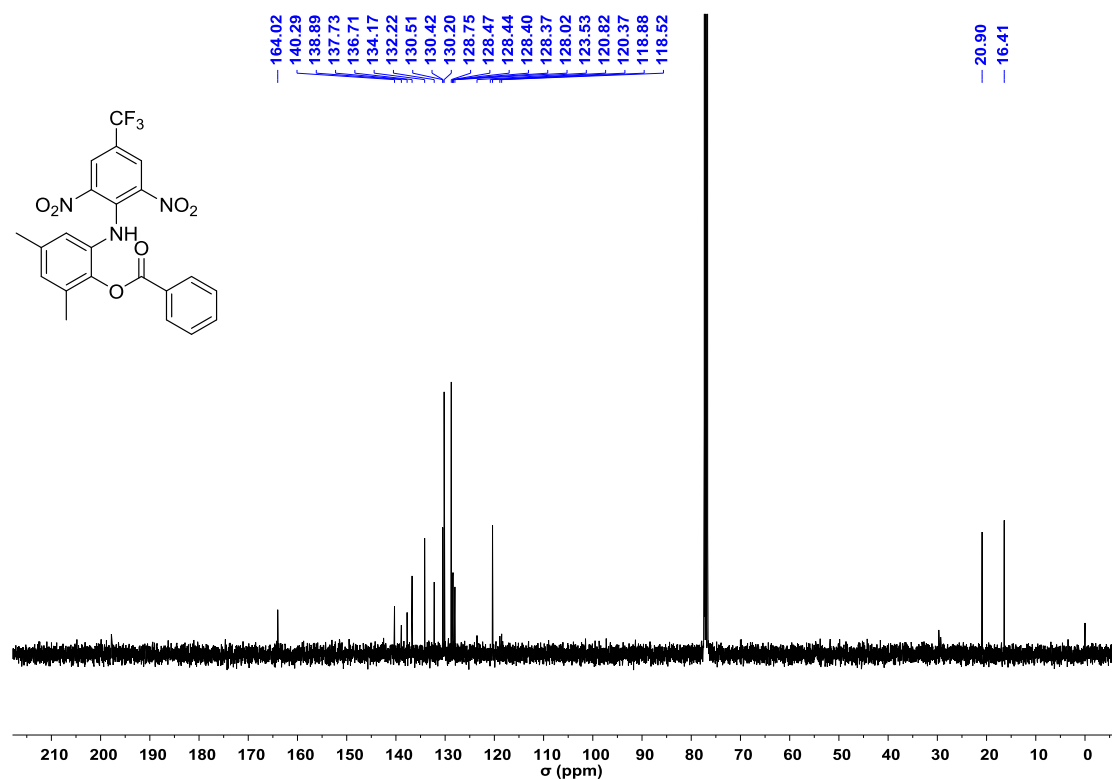
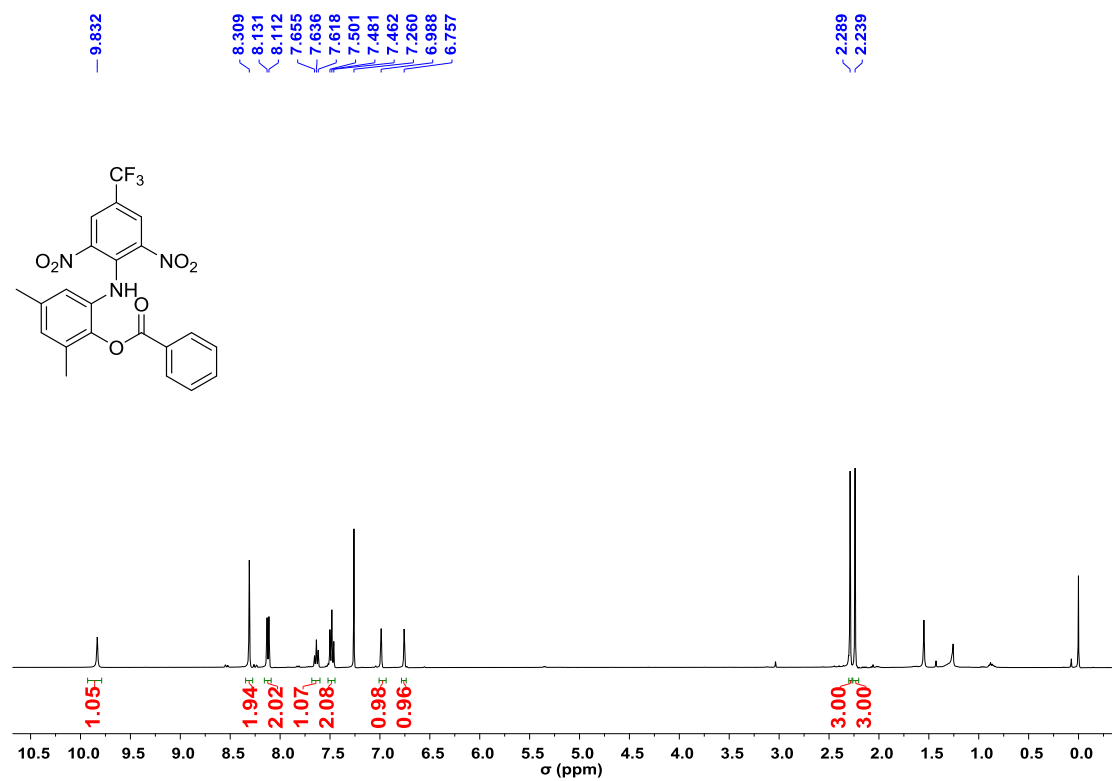
*N*-(2,4-Dinitrophenoxy)-*N*-methylbenzamide (**9**)



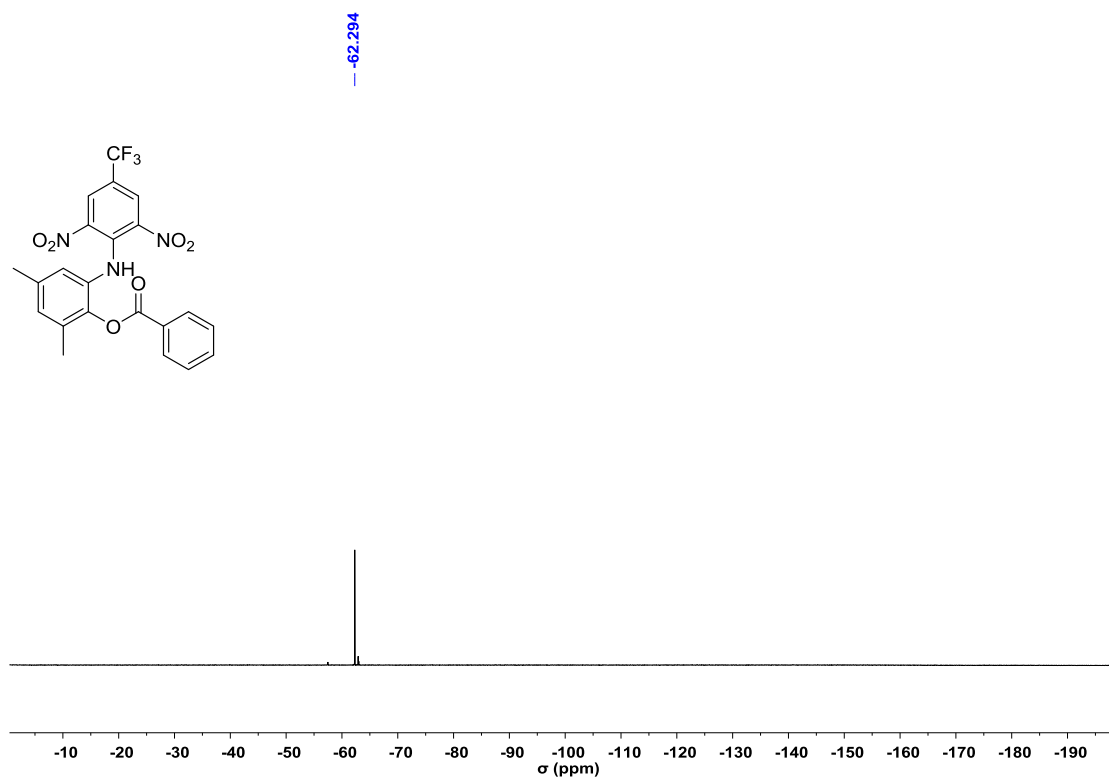
### Copies of NMR spectra of product 12

$^1\text{H}$  NMR (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) in  $\text{CDCl}_3$

2-((2,6-Dinitro-4-(trifluoromethyl)phenyl)amino)-4,6-dimethylphenyl benzoate (**12eg**)



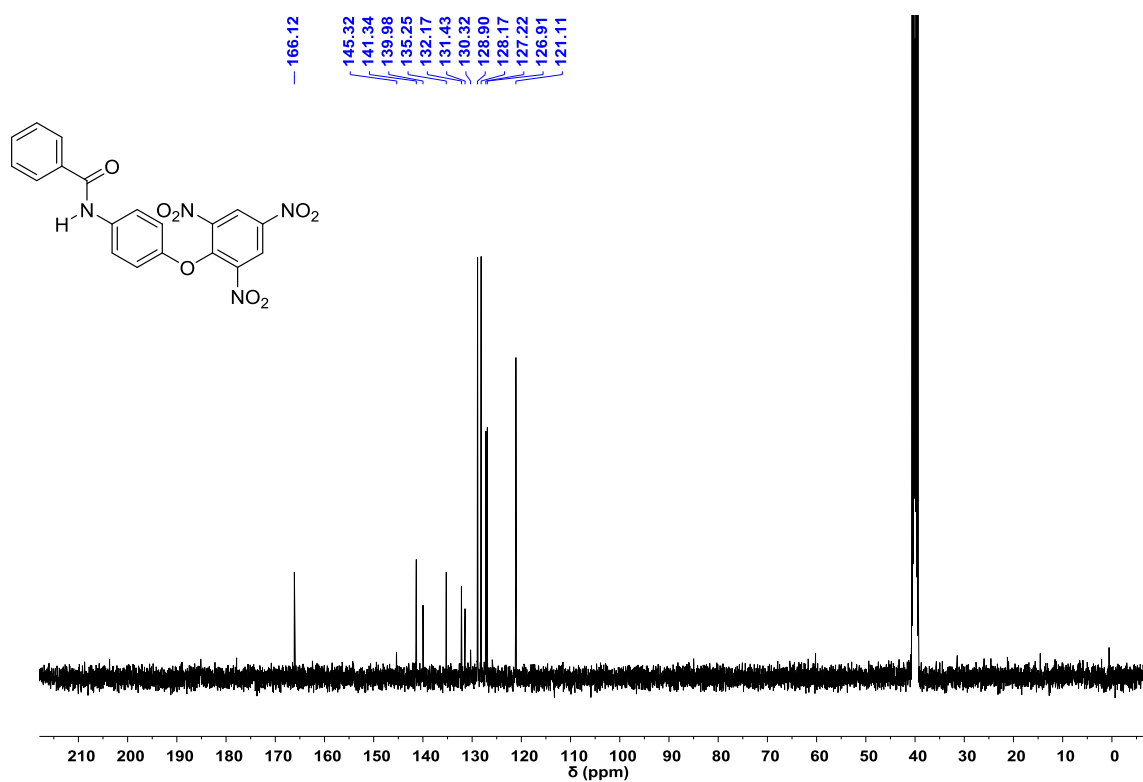
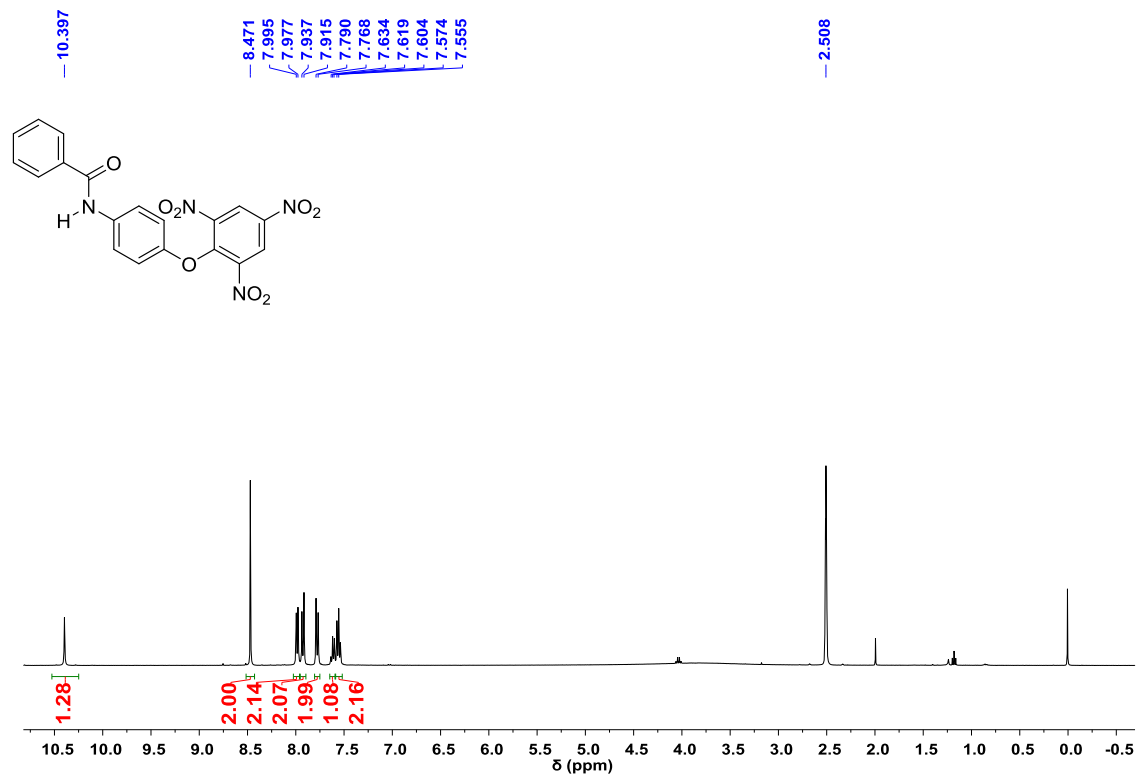
$^{19}\text{F}$  NMR (376 MHz) in  $\text{CDCl}_3$



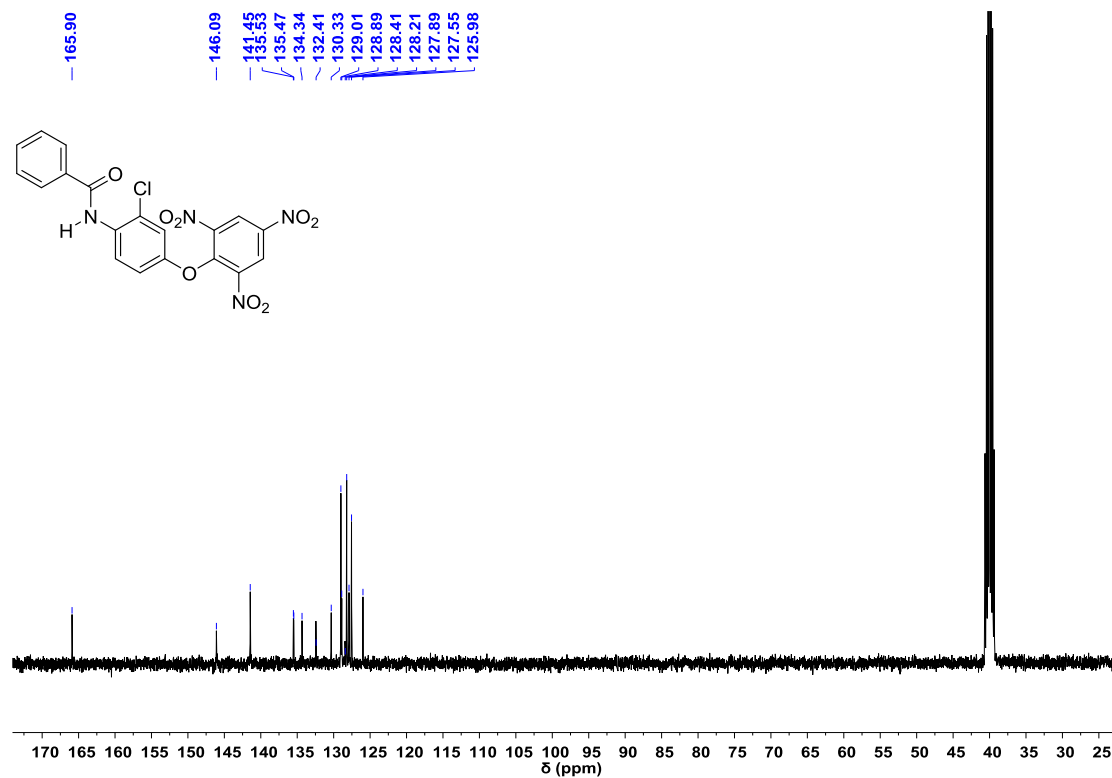
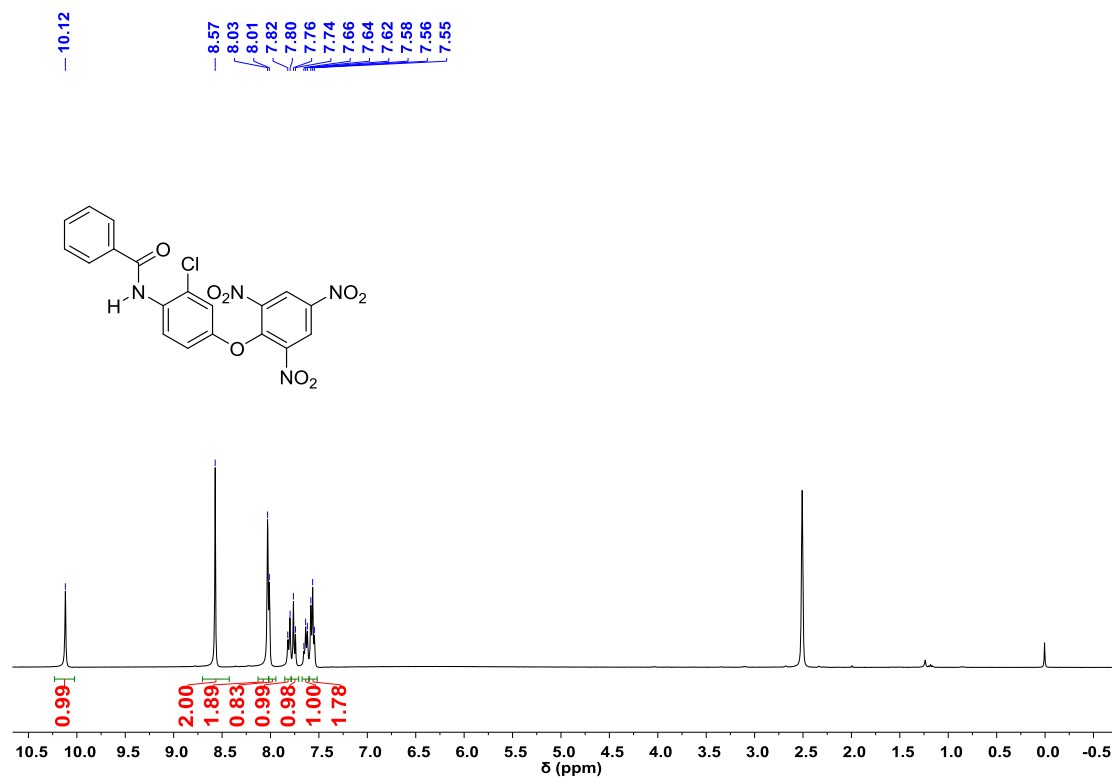
## Copies of NMR spectra of products 16

$^1\text{H}$  NMR (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) in  $\text{DMSO-}d_6$

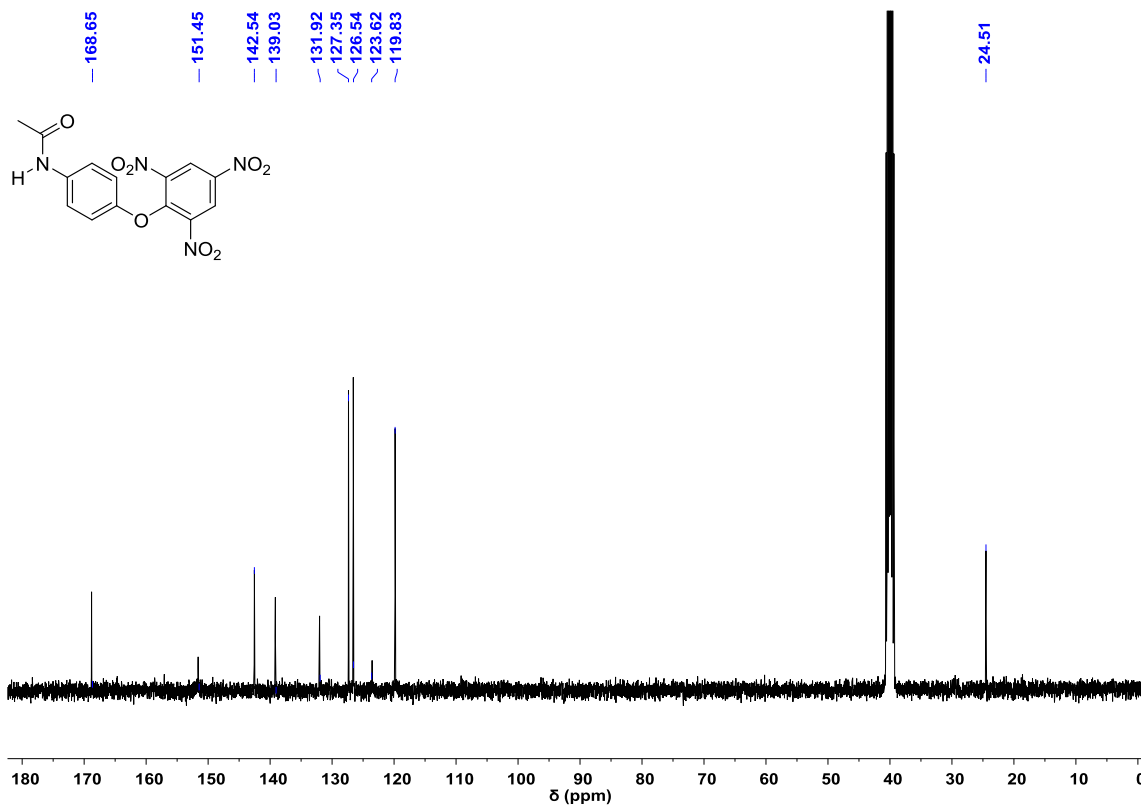
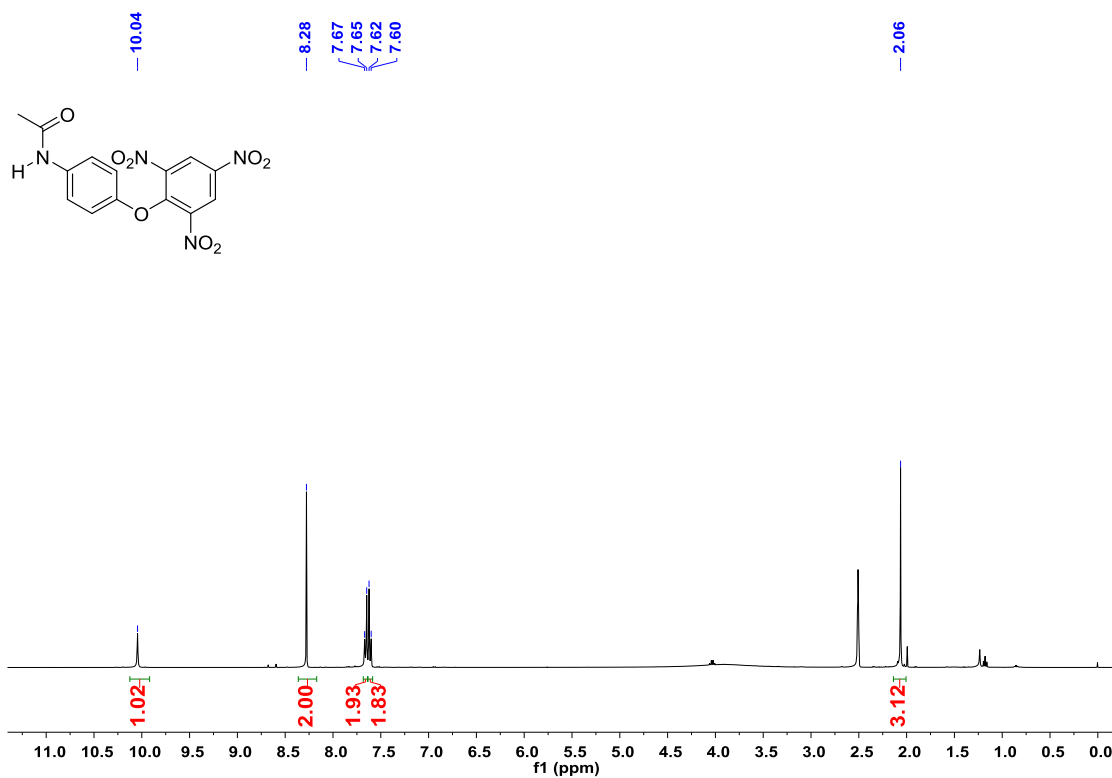
*N*-(4-(2,4,6-Trinitrophenoxy)phenyl)benzamide (**16a**)



*N*-(2-Chloro-4-(2,4,6-trinitrophenoxy)phenyl)benzamide (**16b**)



*N*-(4-(2,4,6-Trinitrophenoxy)phenyl)acetamide (**16c**)

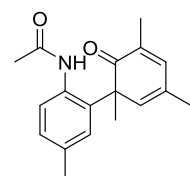
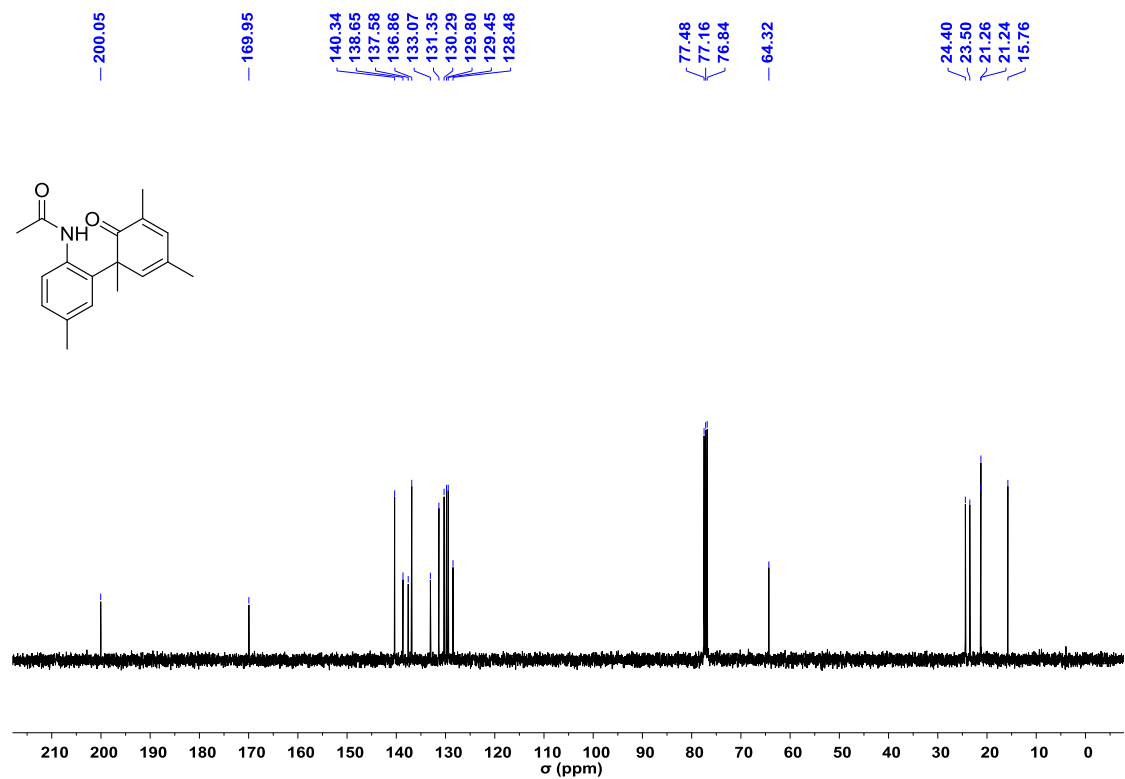
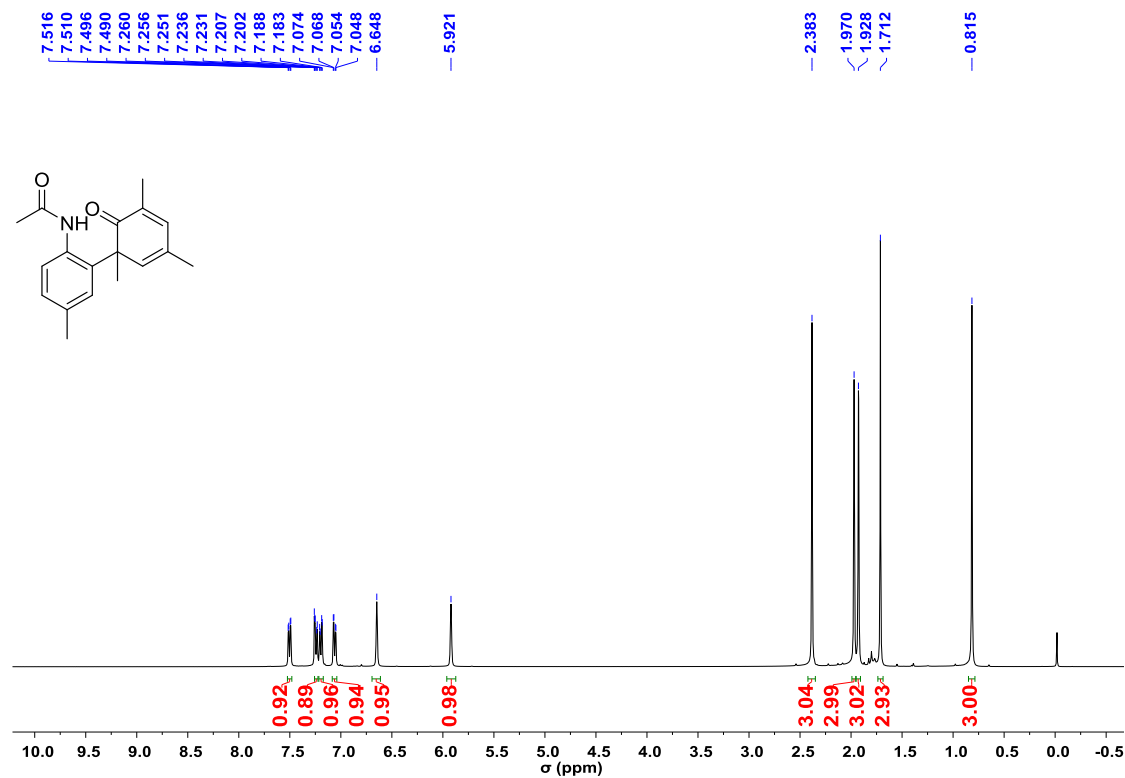




### Copies of NMR spectra of product 19

$^1\text{H}$  NMR (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) in  $\text{CDCl}_3$

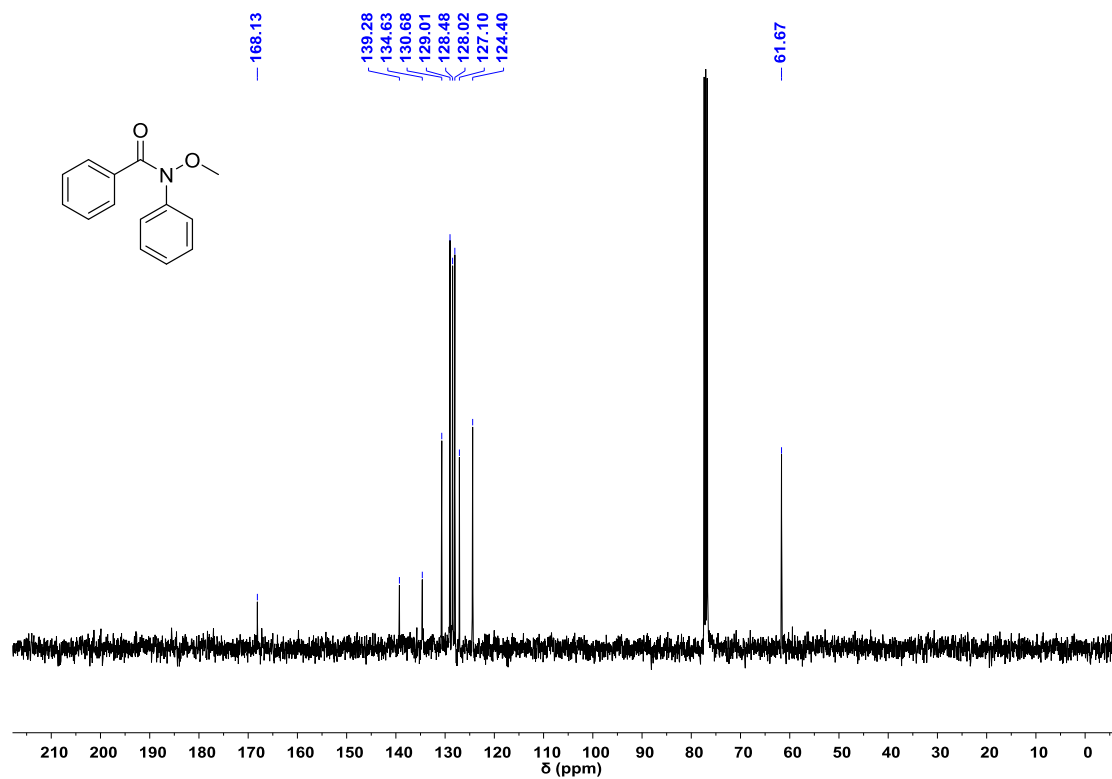
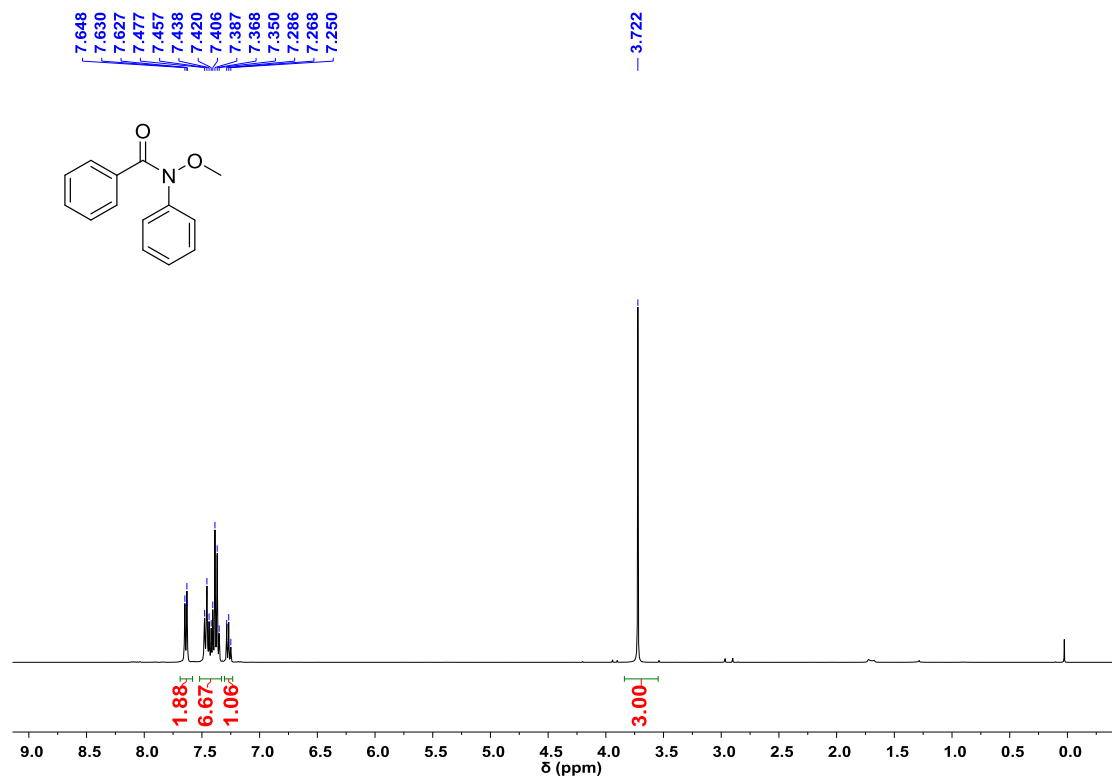
*N*-(1',3',5,5'-Tetramethyl-2'-oxo-1',2'-dihydro-[1,1'-biphenyl]-2-yl)acetamide (**19**)



## Copies of NMR spectra of product 21

$^1\text{H}$  NMR (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) in  $\text{CDCl}_3$

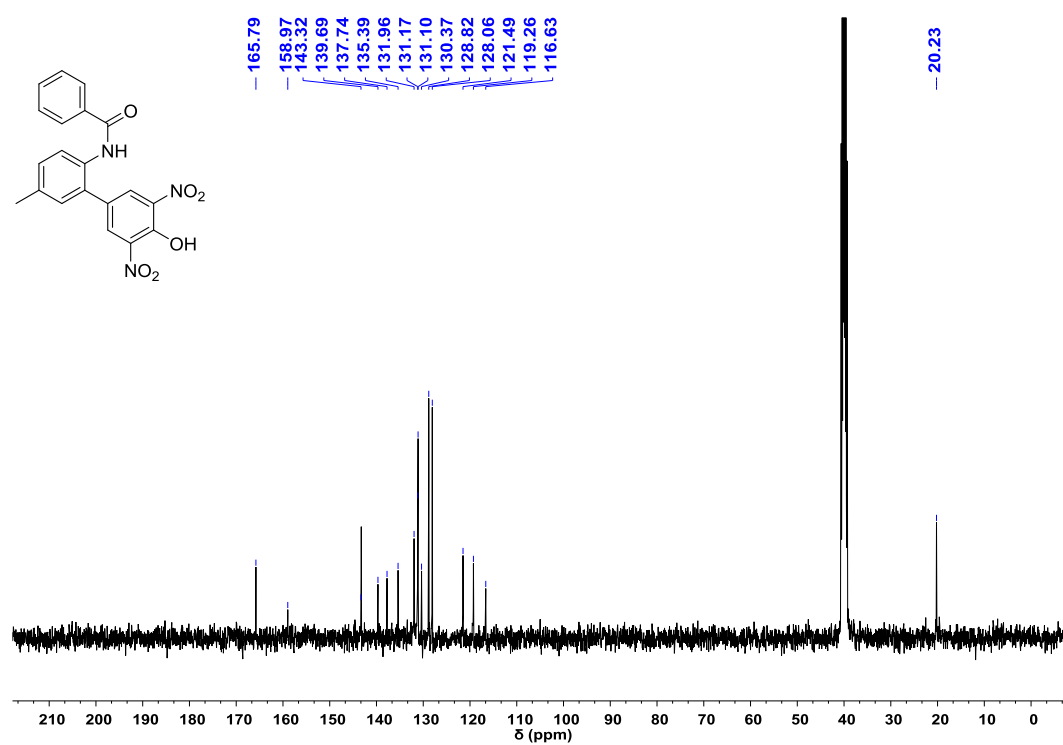
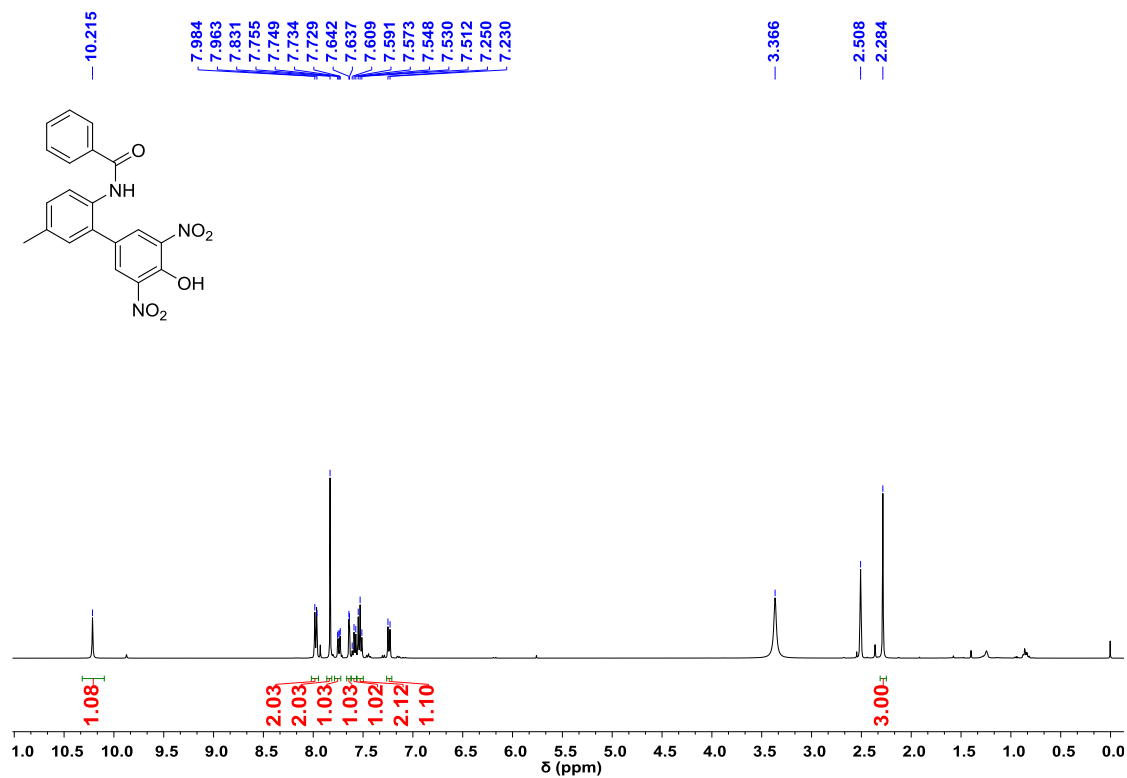
### *N*-Methoxy-*N*-phenylbenzamide (**21**)



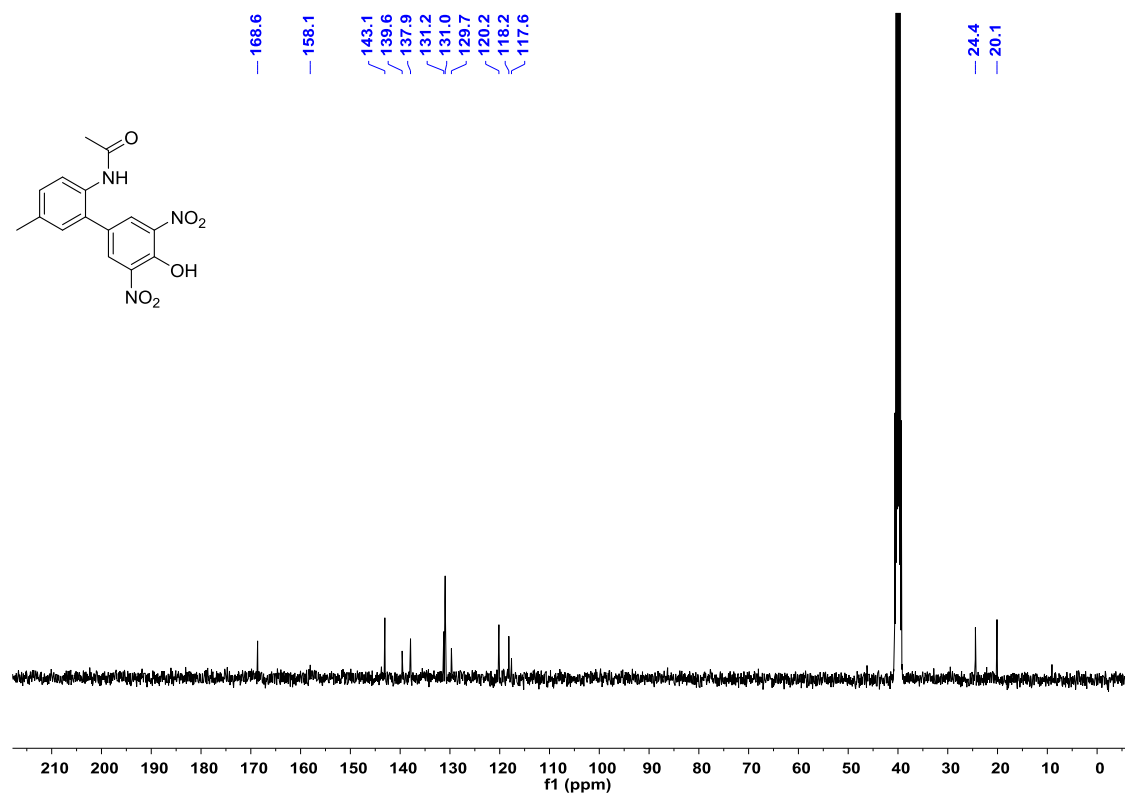
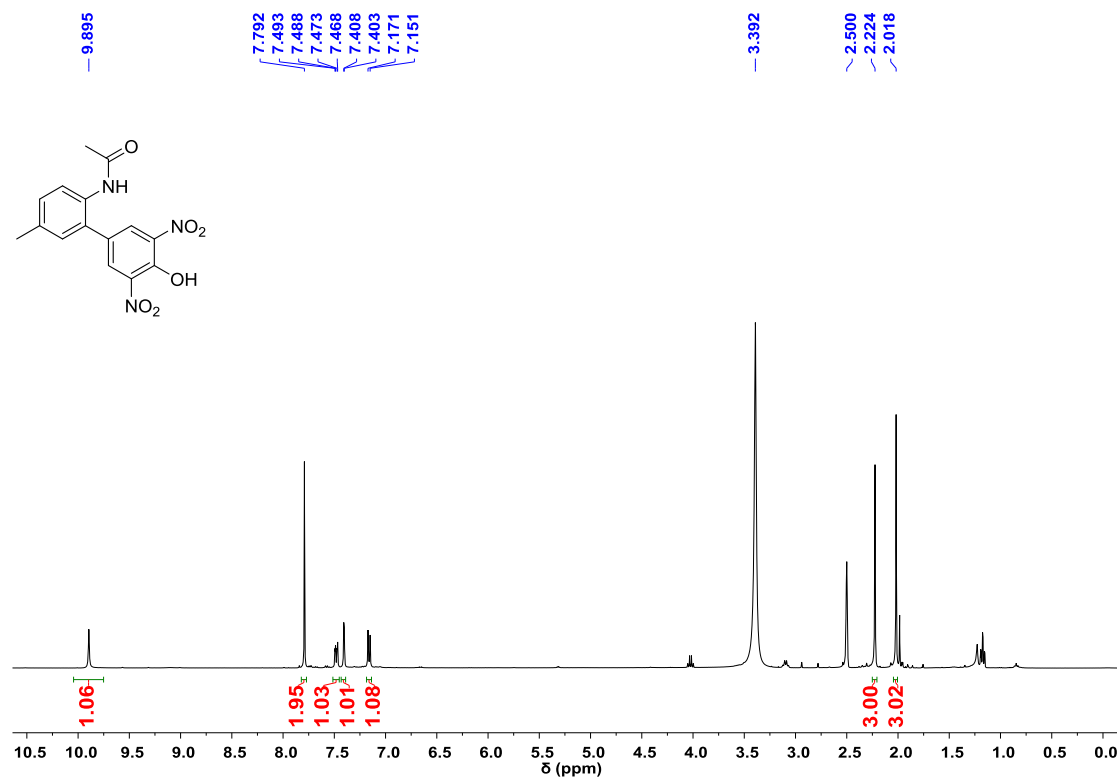
### Copies of NMR spectra of products 25

<sup>1</sup>H NMR (400 MHz) and <sup>13</sup>C NMR (101 MHz) in DMSO-*d*<sub>6</sub>

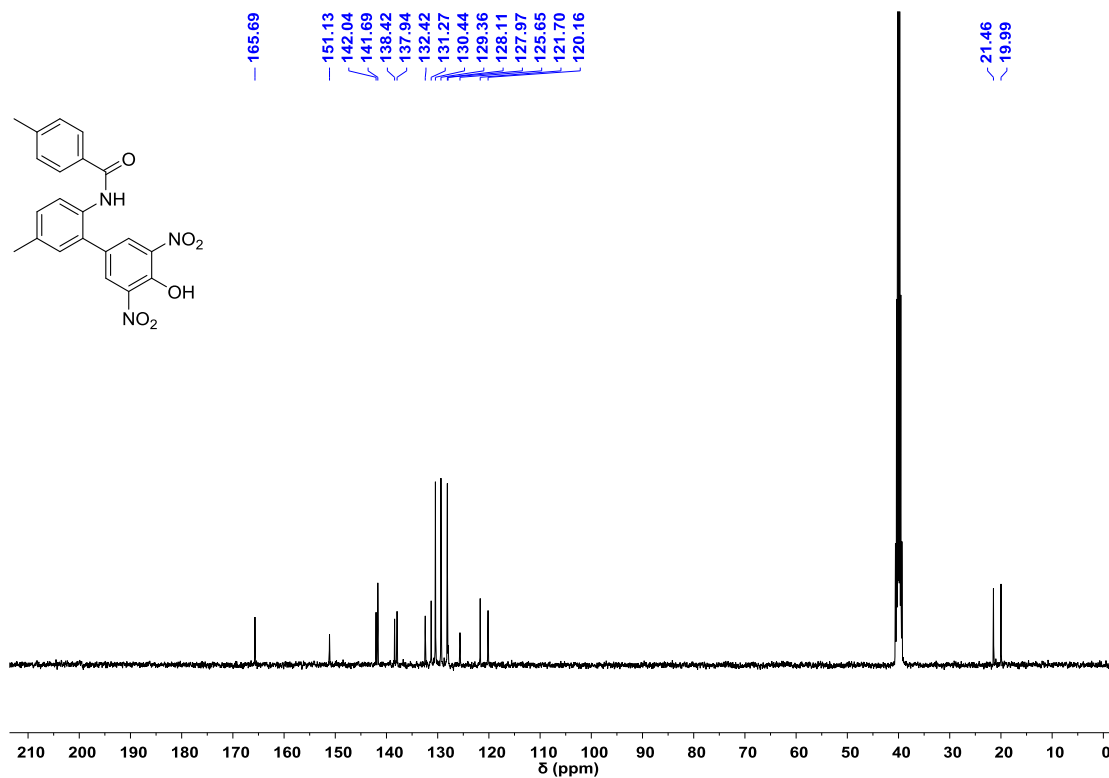
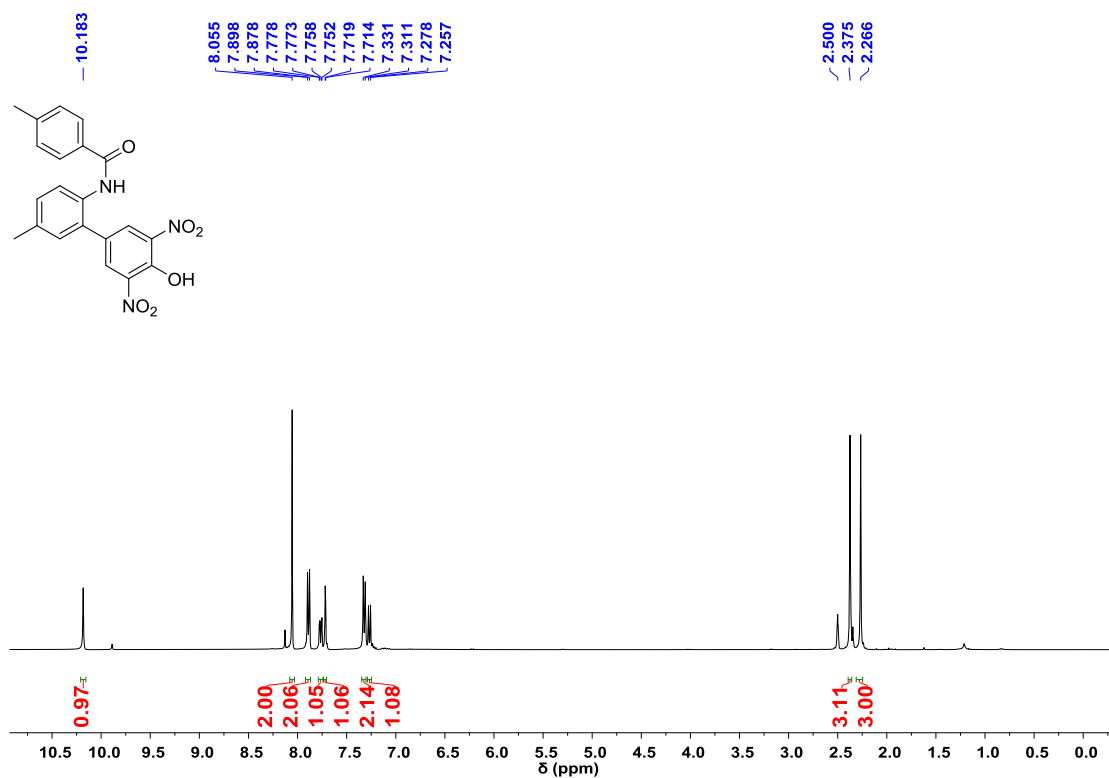
*N*-(4'-Hydroxy-5-methyl-3',5'-dinitro-[1,1'-biphenyl]-2-yl)benzamide (**25a**)



*N*-(4'-Hydroxy-5-methyl-3',5'-dinitro-[1,1'-biphenyl]-2-yl)acetamide (**25b**)

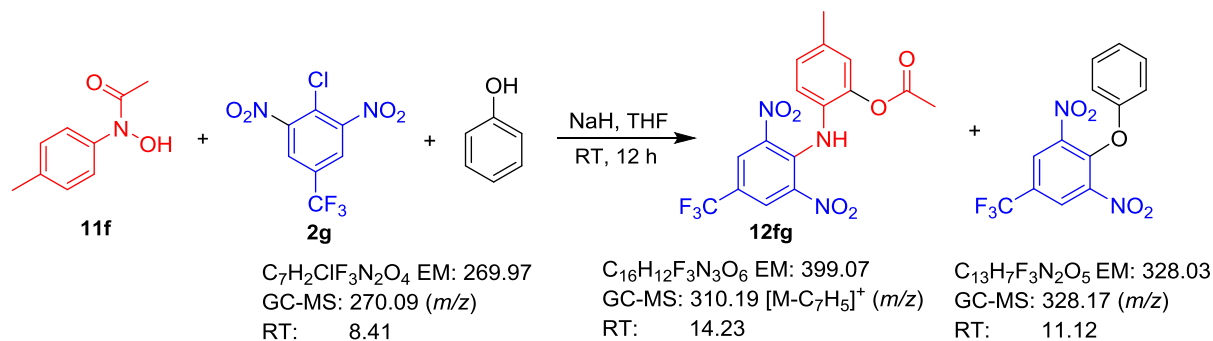


*N*-(4'-Hydroxy-5-methyl-3',5'-dinitro-[1,1'-biphenyl]-2-yl)-4-methylbenzamide (**25c**)



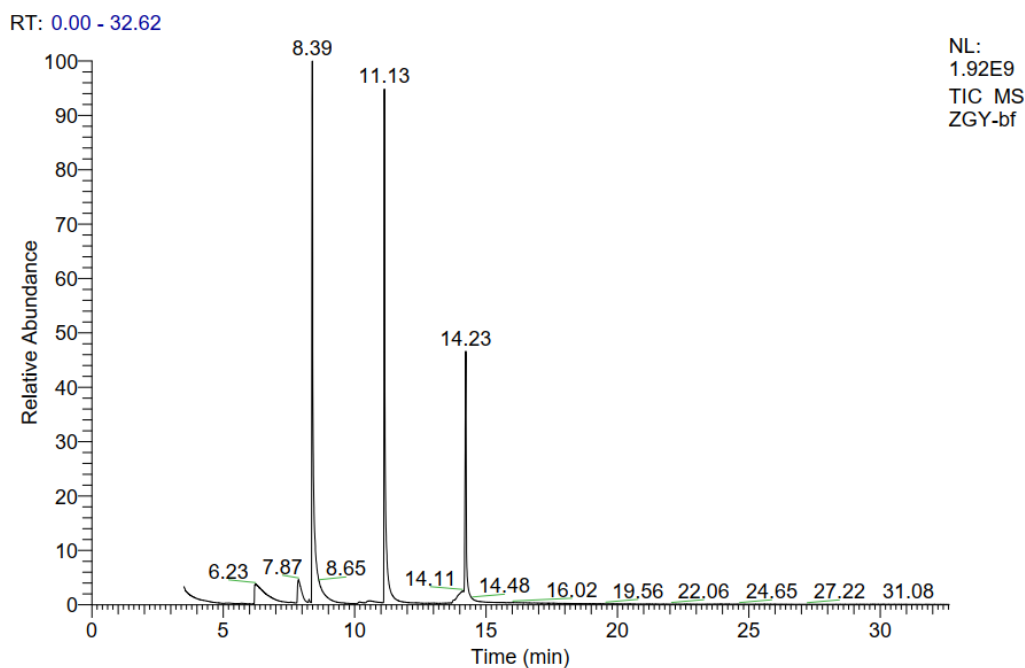
## Control experiments

GC-MS analysis for the reaction of **11f** and **2g** with phenol as additive

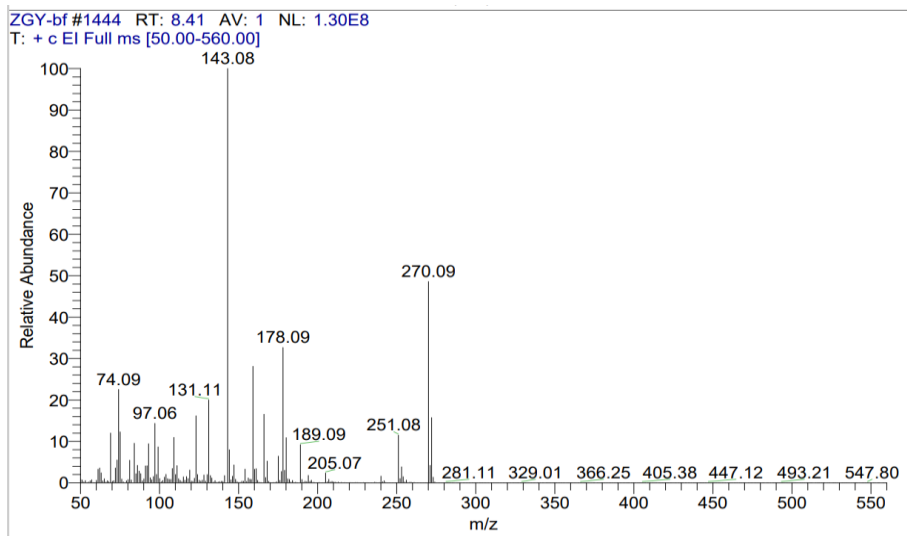


For product **12fg**, only its fragment ions at 310  $m/z$ , 293  $m/z$ , 263  $m/z$ , 234  $m/z$ , 194  $m/z$ , 102  $m/z$ , 89  $m/z$  were observed in GC-MS analysis at RT 14.23. It was verified by injection of the authentic sample **12fg**, showing the same fragment ions and RT value.

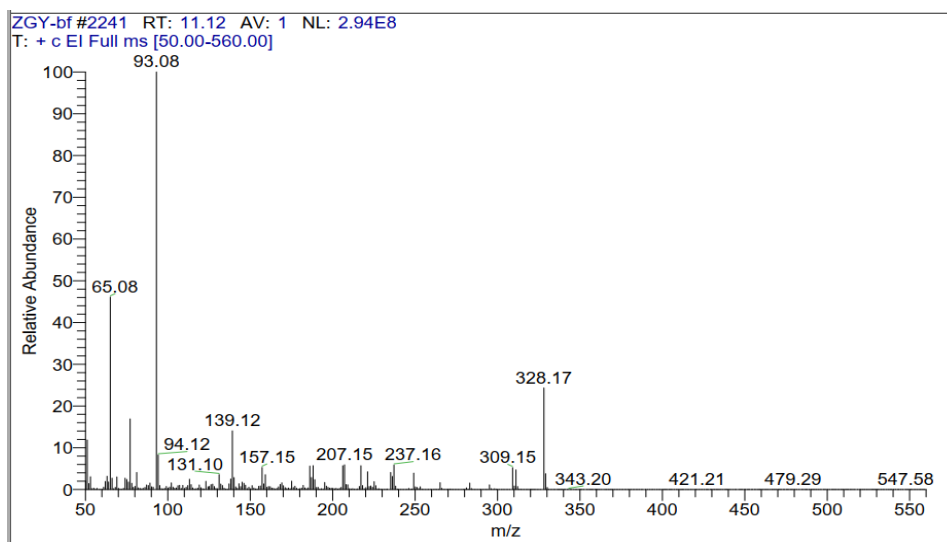
## GC profile



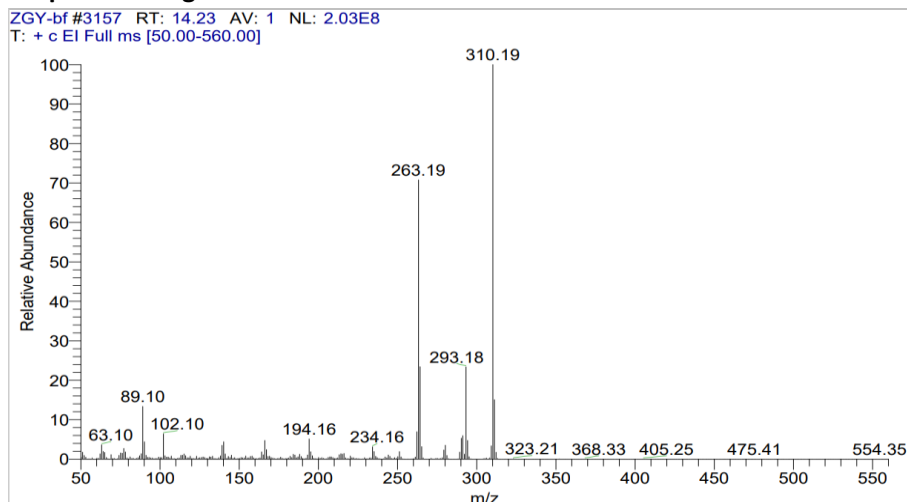
### MS spectrum of compound 2g at RT 8.41 min.



### MS spectrum of compound phenyl 2,6-dinitro-4-trifluoromethylphenyl ether at RT 11.12 min.



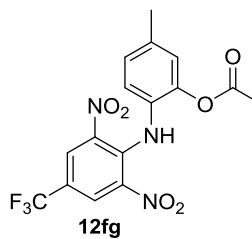
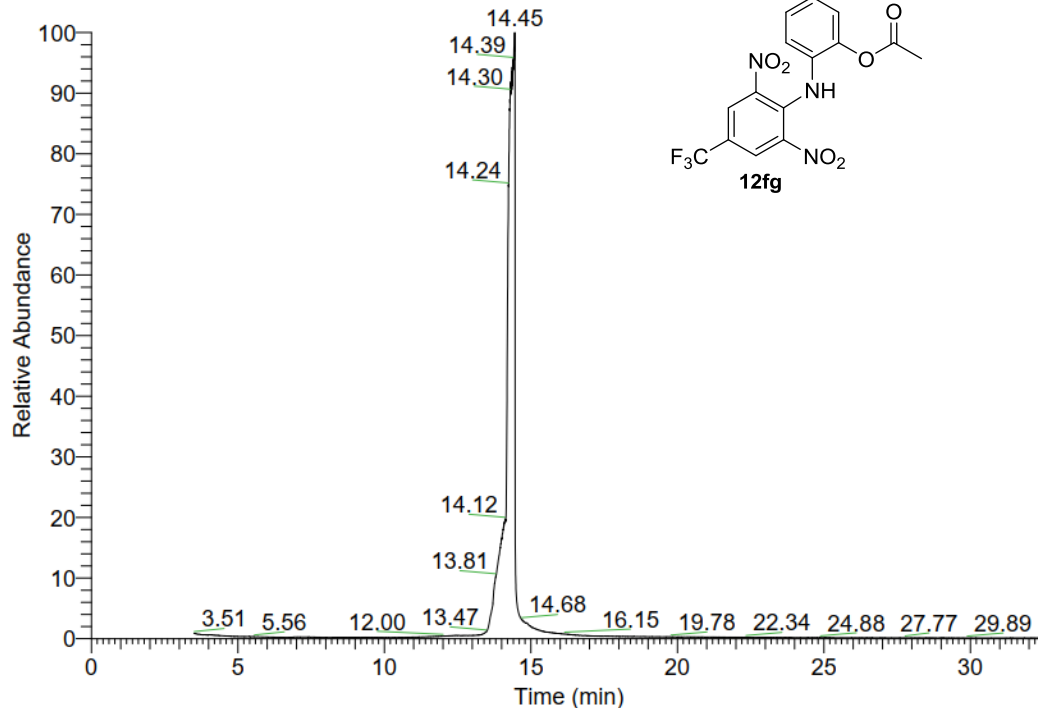
### MS spectrum of product 12fg at RT 14.23 min.



### GC-MS analysis of the authentic sample 12fg

#### GC profile

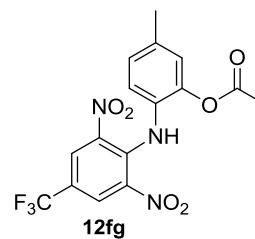
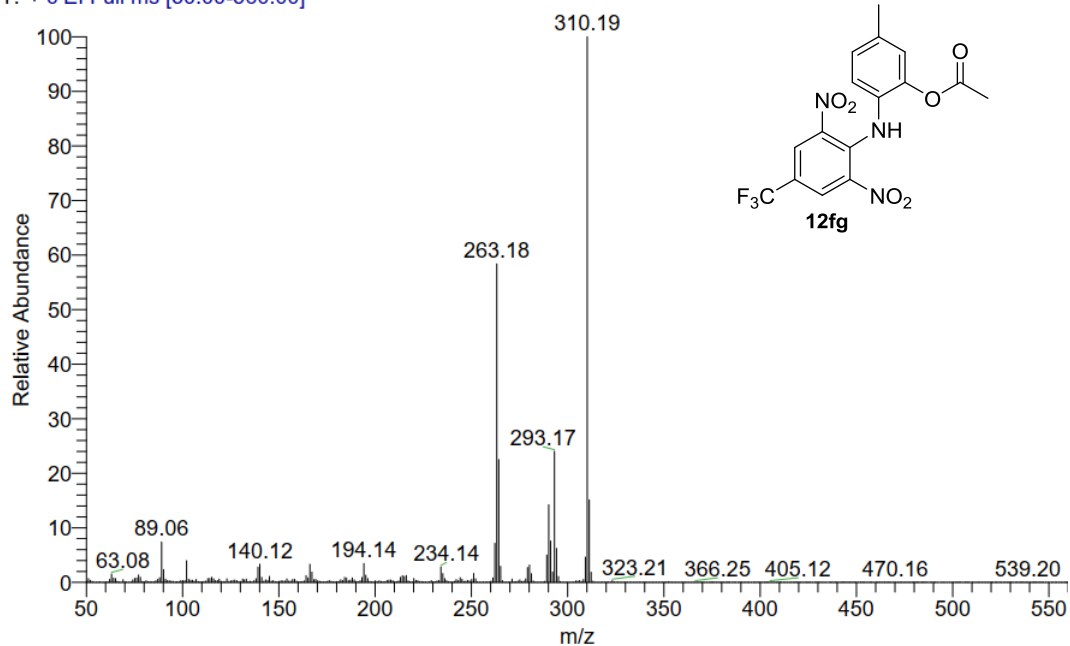
RT: 0.00 - 32.61



NL:  
1.94E9  
TIC MS  
ZGY-  
YIXIANJI

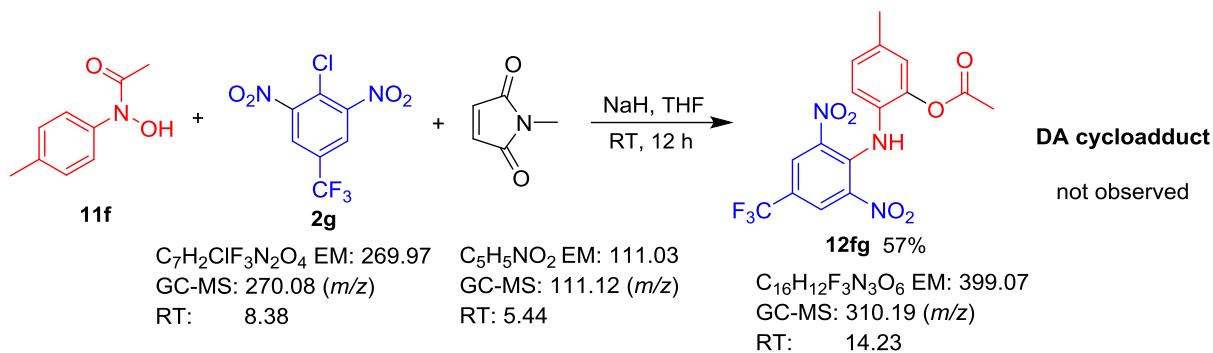
#### MS spectrum of authentic sample 12fg at RT 14.36 min.

ZGY-YIXIANJI #3194 RT: 14.36 AV: 1 NL: 4.71E8  
T: + c EI Full ms [50.00-560.00]



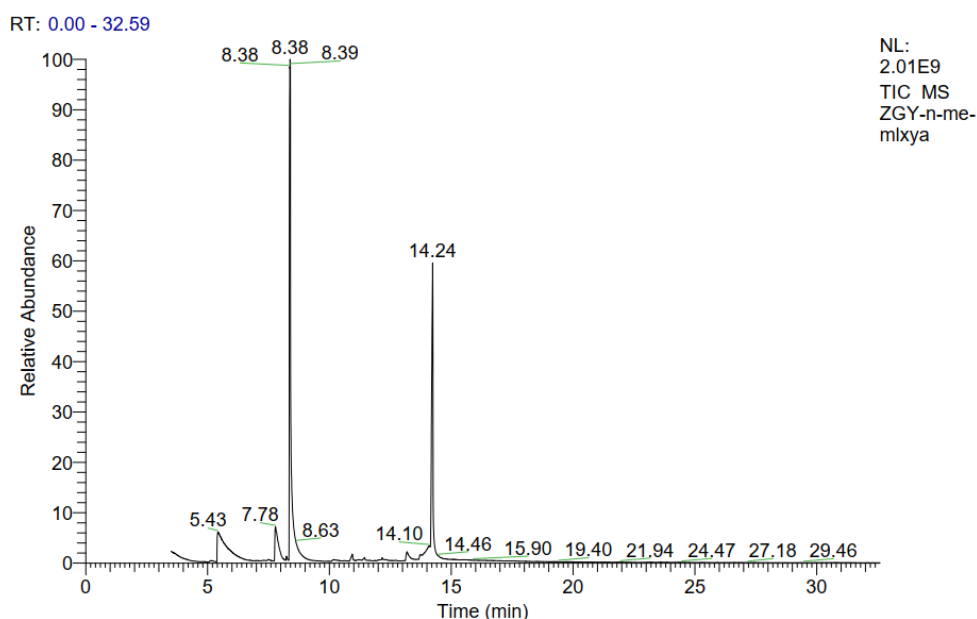


GC-MS analysis for the reaction of **11f** and **2g** with *N*-methylmaleimide as additive

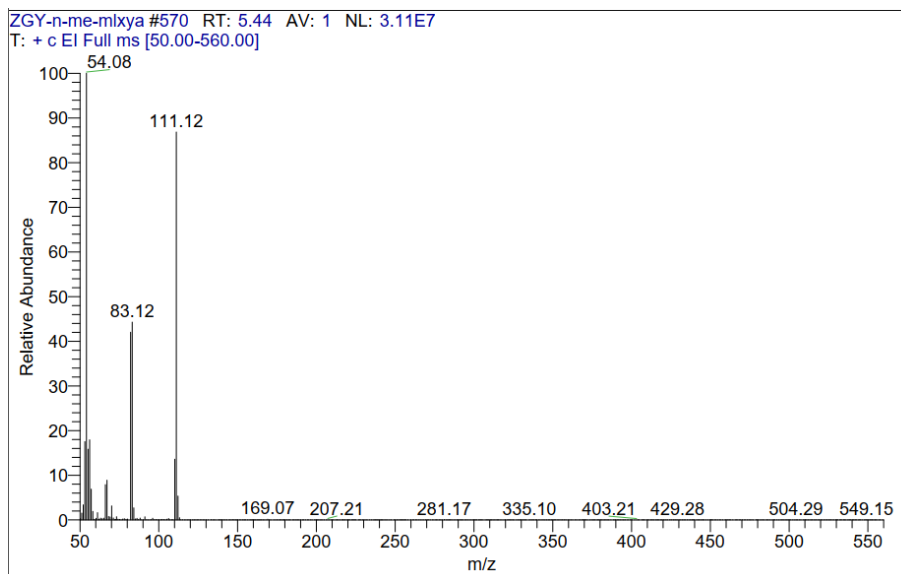


For product **12fg**, the same as that in the above reaction.

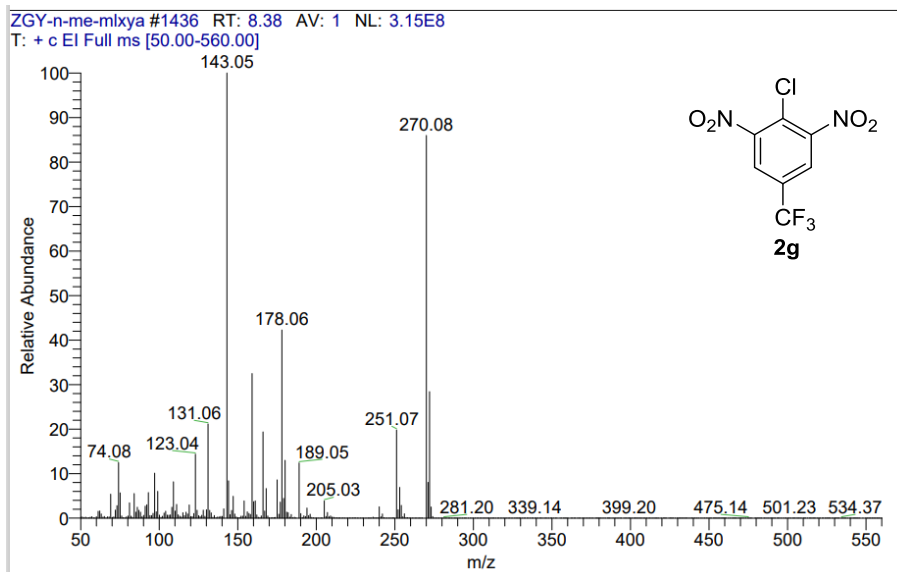
### GC profile



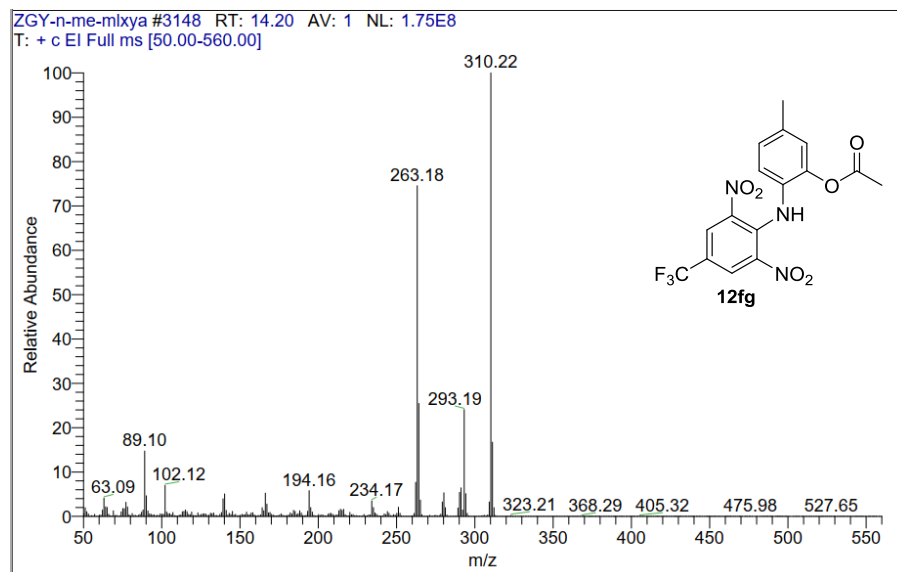
### MS spectrum of *N*-methylmaleimide at RT 5.44 min.



**MS spectrum of compound 2g at RT 8.38 min.**



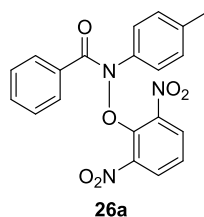
**MS spectrum of product 12fg at RT 14.20 min.**



**DFT calculation****Table 1S.** Sum of electronic and zero-point energies ( $E$ , in Hartree), sum of electronic and thermal enthalpies ( $H$ , in Hartree), and sum of electronic and thermal free energies ( $G$ , in Hartree) for the rearrangement of **26a**.Relative energies ( $\Delta E$ ,  $\Delta H$ ,  $\Delta G$  and  $\Delta G_{sol}$  in DMSO) at 298 K are reported in kcal/mol.

Structure	E	H	G	Gsol+ZPC	$\Delta E_o$	$\Delta H$	$\Delta G$	$\Delta G_{sol}$
<b>26a</b>	-1386.273267	-1386.247555	-1386.331619	-1386.365822	0.0	0.0	0.0	0.0
<b>TS-A-1</b>	-1386.25140	-1386.226073	-1386.306439	-1386.354773	13.7	13.5	15.8	6.9
<b>Int-A-1</b>	-1386.265228	-1386.239817	-1386.320821	-1386.374788	5.0	4.9	6.8	-5.6
<b>TS-A-2</b>	-1386.238077	-1386.212153	-1386.295935	-1386.346650	22.1	22.2	22.4	12.0
<b>Int-2</b>	-1386.266742	-1386.240722	-1386.326935	-1386.403929	4.1	4.3	2.9	-23.9
<b>TS-AB-1</b>	-1386.250729	-1386.225386	-1386.307086	-1386.362143	14.1	13.9	15.4	2.3
<b>TS-B-1</b>	-1386.243241	-1386.217909	-1386.300072	-1386.356097	18.8	18.6	19.8	6.1
<b>Int-B-1</b>	-1386.257151	-1386.231496	-1386.316224	-1386.383258	10.1	10.1	9.7	-10.9
<b>TS-B-2</b>	-1386.223795	-1386.197496	-1386.285355	-1386.342530	31.0	31.4	29.0	14.6
<b>25a</b>	-1386.362278	-1386.336756	-1386.420499	-1386.468999	-55.9	-56.0	-55.8	-64.7
<b>TS-C-1</b>	-1386.235584	-1386.209469	-1386.294484	-1386.353994	23.6	23.9	23.3	7.4
<b>Int-C-1</b>	-1386.290798	-1386.264776	-1386.349038	-1386.390087	-11.0	-10.8	-10.9	-15.2
<b>TS-C-2</b>	-1386.256769	-1386.231387	-1386.312333	-1386.365997	10.4	10.1	12.1	-0.1
<b>TS-D-1</b>	-1386.254551	-1386.228845	-1386.311974	-1386.353635	11.7	11.7	12.3	7.6
<b>Int-D-1</b>	-1386.284377	-1386.258827	-1386.341423	-1386.390889	-7.0	-7.1	-6.2	-15.7
<b>TS-D-2</b>	-1386.253680	-1386.228595	-1386.308636	-1386.355299	12.3	11.9	14.4	6.6
<b>Int-D-2</b>	-1386.262484	-1386.237190	-1386.317593	-1386.365512	6.8	6.5	8.8	0.2
<b>TS-D-3</b>	-1386.257710	-1386.232244	-1386.315639	-1386.371130	9.8	9.6	10.0	-3.3

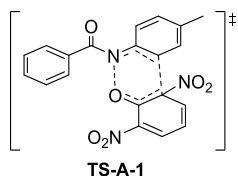
## Coordinates of all stationary points



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.310397	-0.050248	-1.034148
2	6	0	4.213689	0.456827	-1.731598
3	6	0	2.925907	0.005628	-1.446279
4	6	0	2.734234	-0.974172	-0.462036
5	6	0	3.843129	-1.502009	0.215489
6	6	0	5.122696	-1.031448	-0.058032
7	1	0	6.310068	0.314079	-1.254138
8	1	0	4.357625	1.208844	-2.501882
9	1	0	2.085181	0.411317	-1.993952
10	1	0	3.679476	-2.276686	0.956165
11	1	0	5.973685	-1.432767	0.484415
12	6	0	1.422223	-1.608226	-0.141012
13	8	0	1.315069	-2.791931	0.132023
14	7	0	0.257904	-0.822101	-0.078417
15	6	0	-1.058059	-1.342588	-0.290072
16	6	0	-1.600889	-2.214232	0.654494
17	6	0	-1.802510	-0.945560	-1.403076
18	6	0	-2.889071	-2.706014	0.462031
19	1	0	-1.015236	-2.495947	1.520277
20	6	0	-3.098157	-1.428890	-1.563499
21	1	0	-1.371407	-0.262022	-2.126614
22	6	0	-3.659812	-2.322398	-0.642685
23	1	0	-3.309161	-3.389653	1.195164
24	1	0	-3.679364	-1.111607	-2.425347
25	6	0	-5.049001	-2.874464	-0.846320
26	1	0	-5.017928	-3.828340	-1.388948
27	1	0	-5.549373	-3.061219	0.109585
28	1	0	-5.671606	-2.187833	-1.428743
29	8	0	0.385308	0.535981	-0.502712
30	6	0	-0.259882	1.385366	0.343452
31	6	0	-1.024371	2.438152	-0.190812

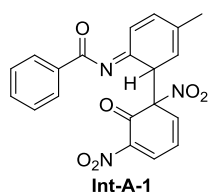
32	6	0	-0.287411	1.231613	1.737719
33	6	0	-1.773169	3.286213	0.625427
34	6	0	-1.054559	2.050284	2.556282
35	6	0	-1.792565	3.093482	2.000281
36	1	0	-2.350951	4.069741	0.151776
37	1	0	-1.051369	1.864448	3.624308
38	1	0	-2.378742	3.747217	2.636036
39	7	0	-1.092748	2.669825	-1.638389
40	8	0	-2.088190	3.259387	-2.059253
41	8	0	-0.159690	2.280182	-2.337366
42	7	0	0.551867	0.227848	2.409324
43	8	0	1.750752	0.248788	2.151171
44	8	0	0.000879	-0.505217	3.226216



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.251785	-0.706154	0.284862
2	6	0	4.322700	0.134972	-0.329608
3	6	0	3.049118	-0.341635	-0.623946
4	6	0	2.695734	-1.657787	-0.299577
5	6	0	3.637847	-2.503838	0.304137
6	6	0	4.910815	-2.027202	0.595669
7	1	0	6.244468	-0.334165	0.523055
8	1	0	4.573785	1.164049	-0.565435
9	1	0	2.326678	0.291882	-1.119590
10	1	0	3.347906	-3.521825	0.541817
11	1	0	5.638146	-2.678935	1.071082
12	6	0	1.338461	-2.188150	-0.566215
13	8	0	1.066532	-3.382421	-0.552283
14	7	0	0.393792	-1.187759	-0.908304
15	6	0	-0.854691	-1.291163	-0.580979
16	6	0	-1.480584	-2.331958	0.223704
17	6	0	-1.742457	-0.212903	-1.081766
18	6	0	-2.827063	-2.461682	0.203011

19	1	0	-0.851291	-3.014883	0.776903
20	6	0	-3.140471	-0.521536	-1.233136
21	1	0	-1.271322	0.417756	-1.829713
22	6	0	-3.685103	-1.593825	-0.591751
23	1	0	-3.301953	-3.252666	0.777040
24	1	0	-3.770593	0.161795	-1.793086
25	6	0	-5.151140	-1.901576	-0.648116
26	1	0	-5.681797	-1.223980	-1.321742
27	1	0	-5.326796	-2.932865	-0.977517
28	1	0	-5.589222	-1.802018	0.353067
29	8	0	0.471946	0.481089	1.205905
30	6	0	-0.176340	1.325567	0.607462
31	6	0	0.438745	2.451750	-0.120931
32	6	0	-1.664395	1.216986	0.384117
33	6	0	-0.265384	3.346666	-0.859661
34	6	0	-2.370600	2.315000	-0.254008
35	6	0	-1.697299	3.298556	-0.901957
36	1	0	0.271842	4.127962	-1.387283
37	1	0	-3.452168	2.287969	-0.224576
38	1	0	-2.235208	4.082010	-1.424527
39	7	0	1.884899	2.639170	-0.016502
40	8	0	2.485930	2.955834	-1.049885
41	8	0	2.398290	2.483876	1.083168
42	7	0	-2.459561	0.586779	1.480475
43	8	0	-1.884624	0.087322	2.435923
44	8	0	-3.687380	0.606807	1.332542

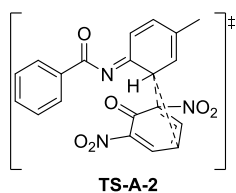


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.219873	-1.830394	0.351985
2	6	0	-4.947693	-0.770373	-0.517748
3	6	0	-3.638079	-0.503488	-0.898092
4	6	0	-2.588440	-1.296598	-0.409358
5	6	0	-2.865738	-2.360260	0.461441

6	6	0	-4.179105	-2.622987	0.840857
7	1	0	-6.244060	-2.036089	0.651105
8	1	0	-5.756319	-0.148609	-0.889998
9	1	0	-3.407183	0.322897	-1.560904
10	1	0	-2.044708	-2.963507	0.829020
11	1	0	-4.392527	-3.444774	1.518209
12	6	0	-1.202198	-0.963345	-0.809379
13	8	0	-0.962222	-0.039096	-1.596043
14	7	0	-0.224968	-1.804296	-0.266681
15	6	0	1.046125	-1.552301	-0.271248
16	6	0	1.728438	-0.250322	-0.721022
17	6	0	1.903796	-2.661475	0.110526
18	6	0	3.188748	-0.417794	-1.041612
19	1	0	1.180519	0.081780	-1.607872
20	6	0	3.232433	-2.654363	-0.124163
21	1	0	1.401127	-3.519552	0.542292
22	6	0	3.899617	-1.524709	-0.759938
23	1	0	3.675535	0.420545	-1.530744
24	1	0	3.833748	-3.520683	0.140057
25	6	0	5.362987	-1.654004	-1.085780
26	1	0	5.544524	-2.508891	-1.749106
27	1	0	5.748404	-0.754727	-1.574309
28	1	0	5.949352	-1.826020	-0.174385
29	8	0	-0.384283	0.448779	1.569160
30	6	0	0.080498	1.169093	0.715845
31	6	0	1.573438	0.987645	0.280759
32	6	0	-0.650471	2.215546	-0.033869
33	6	0	2.186739	2.210502	-0.331427
34	6	0	-0.010521	3.150146	-0.767809
35	6	0	1.431662	3.186116	-0.860220
36	1	0	3.267643	2.261365	-0.360366
37	1	0	-0.605082	3.901996	-1.274698
38	1	0	1.894506	4.034657	-1.353054
39	7	0	2.333867	0.686992	1.576745
40	8	0	2.901745	1.642919	2.101310
41	8	0	2.290960	-0.447574	2.018593
42	7	0	-2.110750	2.300183	0.055878
43	8	0	-2.655895	1.826901	1.044771
44	8	0	-2.693643	2.853027	-0.880957

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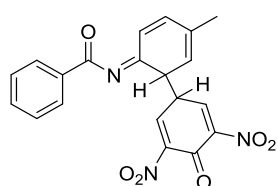


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.825948	2.036584	1.351532
2	6	0	4.359161	0.725561	1.213303
3	6	0	3.193133	0.468005	0.500881
4	6	0	2.483539	1.531990	-0.075854
5	6	0	2.944179	2.851883	0.078218
6	6	0	4.117972	3.098506	0.783645
7	1	0	5.738323	2.230767	1.908648
8	1	0	4.900435	-0.098736	1.667095
9	1	0	2.811808	-0.541991	0.426396
10	1	0	2.386583	3.664471	-0.372428
11	1	0	4.481946	4.116176	0.890332
12	6	0	1.246977	1.240607	-0.835854
13	8	0	1.015048	0.175393	-1.410851
14	7	0	0.371883	2.328862	-0.897303
15	6	0	-0.936831	2.205082	-0.785738
16	6	0	-1.659546	0.970167	-0.565816
17	6	0	-1.695203	3.434701	-0.795904
18	6	0	-3.000570	1.002900	-0.268283
19	1	0	-1.126028	0.039002	-0.657186
20	6	0	-3.035920	3.433100	-0.511838
21	1	0	-1.146269	4.352029	-0.978584
22	6	0	-3.713132	2.220741	-0.220131
23	1	0	-3.517825	0.078935	-0.036890
24	1	0	-3.590466	4.366534	-0.484387
25	6	0	-5.174454	2.219516	0.105742
26	1	0	-5.762618	1.982771	-0.793046
27	1	0	-5.409444	1.454787	0.852944
28	1	0	-5.511186	3.193926	0.470396
29	8	0	0.799314	-1.609452	1.468018
30	6	0	0.056333	-2.028430	0.582497
31	6	0	-1.419160	-2.085989	0.717029
32	6	0	0.504110	-2.435500	-0.769544
33	6	0	-2.264105	-2.425615	-0.318097
34	6	0	-0.368178	-2.743775	-1.792537



35	6	0	-1.750331	-2.739539	-1.582675
36	1	0	-3.331803	-2.443004	-0.132129
37	1	0	0.049697	-2.996083	-2.759390
38	1	0	-2.422592	-3.008557	-2.389701
39	7	0	-2.040303	-1.763314	1.992964
40	8	0	-3.186791	-1.279642	1.956643
41	8	0	-1.423173	-1.997412	3.023943
42	7	0	1.926223	-2.579033	-1.065715
43	8	0	2.698732	-2.753652	-0.123137
44	8	0	2.267030	-2.557685	-2.250260

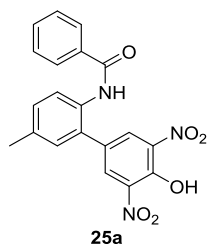


Int-2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.078433	-1.856971	1.385558
2	6	0	4.946847	-2.123631	0.019470
3	6	0	4.244433	-1.242417	-0.795941
4	6	0	3.670283	-0.085887	-0.248827
5	6	0	3.808621	0.181036	1.120985
6	6	0	4.510211	-0.705430	1.934821
7	1	0	5.625951	-2.546681	2.021602
8	1	0	5.390917	-3.019048	-0.405206
9	1	0	4.124315	-1.427359	-1.858115
10	1	0	3.376353	1.087152	1.531303
11	1	0	4.618506	-0.497072	2.995036
12	6	0	2.874468	0.799284	-1.143946
13	8	0	2.795027	0.615467	-2.354625
14	7	0	2.260130	1.883390	-0.505830
15	6	0	1.001445	2.138296	-0.607463
16	6	0	0.003762	1.183758	-1.265506
17	6	0	0.483075	3.356719	-0.012452
18	6	0	-1.388513	1.725949	-1.412049
19	1	0	0.414352	0.922102	-2.246879
20	6	0	-0.820613	3.694770	-0.127161

21	1	0	1.195293	3.982324	0.515198
22	6	0	-1.791316	2.886232	-0.864976
23	1	0	-2.096289	1.106100	-1.956239
24	1	0	-1.175836	4.615588	0.329431
25	6	0	-3.202383	3.396876	-0.974309
26	1	0	-3.228542	4.384278	-1.451773
27	1	0	-3.829883	2.717846	-1.557541
28	1	0	-3.654020	3.508173	0.019449
29	8	0	-3.370482	-2.121573	1.177313
30	6	0	-2.460169	-1.493278	0.679681
31	6	0	-1.930319	-1.752500	-0.691146
32	6	0	-1.667174	-0.462518	1.408332
33	6	0	-0.812565	-1.203191	-1.180662
34	6	0	-0.542069	0.087630	0.939387
35	6	0	-0.035259	-0.172473	-0.437663
36	1	0	-0.461937	-1.489928	-2.168213
37	1	0	0.007720	0.785432	1.562659
38	1	0	1.005733	-0.517843	-0.366868
39	7	0	-2.679905	-2.683863	-1.551147
40	8	0	-2.026713	-3.463577	-2.242639
41	8	0	-3.899124	-2.575410	-1.539791
42	7	0	-2.144470	-0.031599	2.733092
43	8	0	-3.352645	0.120167	2.857222
44	8	0	-1.294826	0.187415	3.595838

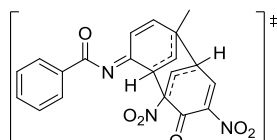


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.020447	-2.628764	-0.633911
2	6	0	-3.037874	-3.545490	-0.258794
3	6	0	-1.691961	-3.251073	-0.467838
4	6	0	-1.319929	-2.040164	-1.064159
5	6	0	-2.313215	-1.138732	-1.467101
6	6	0	-3.656202	-1.425952	-1.243046

7	1	0	-5.067787	-2.851870	-0.453360
8	1	0	-3.318626	-4.487885	0.201699
9	1	0	-0.940740	-3.984912	-0.186922
10	1	0	-2.004453	-0.212241	-1.938715
11	1	0	-4.418859	-0.711184	-1.537433
12	6	0	0.097496	-1.588383	-1.232289
13	8	0	0.421110	-0.729102	-2.041399
14	7	0	1.002176	-2.129724	-0.337188
15	6	0	2.269376	-1.526277	-0.077294
16	6	0	2.349087	-0.175849	0.323039
17	6	0	3.434792	-2.277880	-0.203228
18	6	0	3.607399	0.387912	0.546948
19	6	0	4.677888	-1.703444	0.055684
20	1	0	3.359366	-3.312892	-0.522238
21	6	0	4.784907	-0.357224	0.419964
22	1	0	3.665364	1.429165	0.854509
23	1	0	5.576949	-2.306046	-0.042071
24	6	0	6.131272	0.283161	0.650714
25	1	0	6.522887	0.719335	-0.277348
26	1	0	6.070158	1.089228	1.388912
27	1	0	6.866086	-0.447342	1.003558
28	8	0	-2.611861	2.556193	0.515254
29	6	0	-1.418230	1.982922	0.530848
30	6	0	-0.298967	2.475366	-0.198063
31	6	0	-1.185687	0.795749	1.264954
32	6	0	0.925036	1.804692	-0.236376
33	6	0	0.043216	0.154117	1.244355
34	6	0	1.111910	0.626050	0.474455
35	1	0	1.707323	2.199707	-0.871223
36	1	0	0.137020	-0.754884	1.821722
37	7	0	-0.412948	3.688178	-0.985226
38	8	0	0.579083	4.124369	-1.552141
39	8	0	-1.530147	4.251764	-1.053056
40	7	0	-2.249807	0.155239	2.047479
41	8	0	-3.201772	0.836217	2.410730
42	8	0	-2.103773	-1.044094	2.301049
43	1	0	-2.535226	3.339291	-0.090737
44	1	0	0.644265	-2.770511	0.357533

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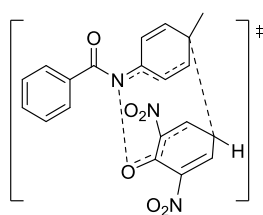


TS-AB-1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.697459	-1.344959	0.383313
2	6	0	5.471735	-1.286530	-0.995178
3	6	0	4.449259	-0.489241	-1.497095
4	6	0	3.650200	0.259838	-0.622356
5	6	0	3.879118	0.198968	0.758975
6	6	0	4.899798	-0.604873	1.258146
7	1	0	6.494250	-1.971172	0.775236
8	1	0	6.090971	-1.866205	-1.673485
9	1	0	4.247710	-0.432110	-2.561297
10	1	0	3.250593	0.770474	1.431592
11	1	0	5.070036	-0.657983	2.329223
12	6	0	2.554690	1.074172	-1.200173
13	8	0	2.350507	1.174347	-2.404830
14	7	0	1.819341	1.831519	-0.264004
15	6	0	0.530566	1.946201	-0.312708
16	6	0	-0.369903	1.193416	-1.197549
17	6	0	-0.087747	2.910671	0.595748
18	6	0	-1.710136	1.370847	-1.128169
19	1	0	0.073941	0.542025	-1.939165
20	6	0	-1.427298	3.038100	0.680495
21	1	0	0.589122	3.516521	1.188811
22	6	0	-2.329310	2.190939	-0.102776
23	1	0	-2.364602	0.835123	-1.809251
24	1	0	-1.874709	3.761664	1.357662
25	6	0	-3.705111	2.748357	-0.395412
26	1	0	-3.600711	3.607220	-1.070714
27	1	0	-4.343365	2.013535	-0.892159
28	1	0	-4.204986	3.102949	0.511357
29	8	0	-1.054597	-2.651440	-0.277402
30	6	0	-1.581926	-1.690372	0.252341
31	6	0	-0.887216	-0.756277	1.185236
32	6	0	-3.004433	-1.312648	0.052795
33	6	0	-1.494848	0.289910	1.794510
34	6	0	-3.572037	-0.207622	0.585776

35	6	0	-2.795148	0.721398	1.368941
36	1	0	-0.932494	0.877821	2.508966
37	1	0	-4.612383	0.005653	0.367181
38	1	0	-3.336845	1.401182	2.019201
39	7	0	0.534963	-0.971399	1.468293
40	8	0	0.944954	-0.673415	2.592649
41	8	0	1.227120	-1.383798	0.545638
42	7	0	-3.844978	-2.161190	-0.793356
43	8	0	-3.718897	-3.373415	-0.689855
44	8	0	-4.638846	-1.579901	-1.542306

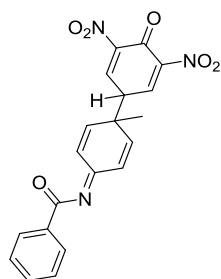


**TS-B-1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.373578	0.109541	-0.918859
2	6	0	-5.431121	0.511168	-1.867783
3	6	0	-4.075546	0.511345	-1.546621
4	6	0	-3.659825	0.111263	-0.269415
5	6	0	-4.608817	-0.294236	0.679421
6	6	0	-5.961106	-0.294549	0.354506
7	1	0	-7.430165	0.106883	-1.172205
8	1	0	-5.752841	0.816995	-2.859085
9	1	0	-3.330364	0.804573	-2.277615
10	1	0	-4.260990	-0.605493	1.658616
11	1	0	-6.695598	-0.610868	1.089422
12	6	0	-2.228714	0.122463	0.126492
13	8	0	-1.835079	-0.303639	1.207707
14	7	0	-1.339931	0.585299	-0.856493
15	6	0	-0.313543	1.303173	-0.529327
16	6	0	-0.092373	1.956334	0.767525
17	6	0	0.727791	1.490012	-1.537169
18	6	0	1.112220	2.479533	1.070284
19	1	0	-0.909490	1.989860	1.476820
20	6	0	1.935280	1.984646	-1.203532

21	1	0	0.504096	1.151369	-2.543027
22	6	0	2.273306	2.338387	0.179505
23	1	0	1.273591	2.957241	2.033690
24	1	0	2.721059	2.049898	-1.951162
25	6	0	3.377996	3.364049	0.348266
26	1	0	3.031005	4.336783	-0.021760
27	1	0	3.656175	3.487260	1.399408
28	1	0	4.271067	3.090566	-0.222395
29	8	0	0.532423	-2.151205	-0.474787
30	6	0	1.434914	-1.510179	0.025798
31	6	0	2.665233	-1.103897	-0.717864
32	6	0	1.411072	-0.945448	1.404318
33	6	0	3.490241	-0.119492	-0.309764
34	6	0	2.237835	0.044053	1.796014
35	6	0	3.187702	0.651549	0.881947
36	1	0	4.328836	0.161764	-0.937995
37	1	0	2.126770	0.438577	2.799408
38	1	0	4.029777	1.152283	1.350993
39	7	0	2.955107	-1.759465	-1.994133
40	8	0	3.454451	-1.059977	-2.882186
41	8	0	2.702552	-2.953441	-2.085595
42	7	0	0.476217	-1.487672	2.402301
43	8	0	0.086142	-2.634512	2.236955
44	8	0	0.202450	-0.766365	3.361993



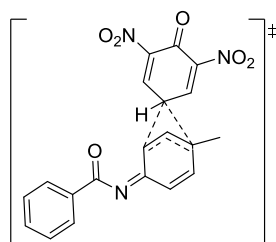
**Int-B-1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	8.226194	-0.057269	0.541989
2	6	0	7.802624	1.083576	-0.146131
3	6	0	6.492531	1.171641	-0.604999
4	6	0	5.595790	0.118151	-0.378348

5	6	0	6.024786	-1.025559	0.308898
6	6	0	7.337411	-1.110236	0.768209
7	1	0	9.249956	-0.125845	0.899254
8	1	0	8.495759	1.900868	-0.322994
9	1	0	6.138584	2.045544	-1.141362
10	1	0	5.327650	-1.840971	0.465852
11	1	0	7.669420	-1.998477	1.297842
12	6	0	4.196085	0.267727	-0.862434
13	8	0	3.830116	1.219868	-1.542839
14	7	0	3.346598	-0.803834	-0.541041
15	6	0	2.151042	-0.608415	-0.092714
16	6	0	1.592386	0.684542	0.327234
17	6	0	1.287580	-1.778188	0.089174
18	6	0	0.320323	0.792995	0.736240
19	1	0	2.243324	1.549962	0.307961
20	6	0	0.012571	-1.667114	0.486520
21	1	0	1.741205	-2.744249	-0.108629
22	6	0	-0.663639	-0.347046	0.748355
23	1	0	-0.050065	1.755734	1.080529
24	1	0	-0.588021	-2.561453	0.632762
25	6	0	-1.412800	-0.389283	2.094941
26	1	0	-0.699876	-0.563379	2.905531
27	1	0	-1.928531	0.555872	2.290220
28	1	0	-2.152098	-1.195956	2.110542
29	8	0	-5.732089	0.291162	0.568477
30	6	0	-4.623469	0.206854	0.084927
31	6	0	-3.693586	1.361749	-0.073719
32	6	0	-3.991780	-1.078450	-0.331318
33	6	0	-2.383013	1.234256	-0.312344
34	6	0	-2.682941	-1.219872	-0.571311
35	6	0	-1.715500	-0.090799	-0.460976
36	1	0	-1.773965	2.129444	-0.373553
37	1	0	-2.303756	-2.202316	-0.830039
38	1	0	-1.086580	-0.072357	-1.360636
39	7	0	-4.248764	2.720737	0.050246
40	8	0	-3.528923	3.573754	0.570416
41	8	0	-5.369930	2.902713	-0.403352
42	7	0	-4.856582	-2.262334	-0.476599
43	8	0	-5.979061	-2.075097	-0.924537
44	8	0	-4.371032	-3.351144	-0.167497

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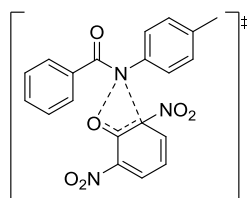
**TS-B-2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	7.229374	-1.208408	1.211530
2	6	0	6.703544	-1.943877	0.144243
3	6	0	5.406150	-1.702165	-0.293223
4	6	0	4.624591	-0.721786	0.335349
5	6	0	5.153826	0.011996	1.407454
6	6	0	6.454473	-0.232550	1.841680
7	1	0	8.242727	-1.399513	1.553245
8	1	0	7.307456	-2.704301	-0.341928
9	1	0	4.974668	-2.259948	-1.117420
10	1	0	4.535107	0.756175	1.895796
11	1	0	6.862212	0.332185	2.674832
12	6	0	3.253673	-0.478442	-0.180038
13	8	0	2.720806	-1.195920	-1.025856
14	7	0	2.583317	0.588550	0.429220
15	6	0	1.737582	1.344020	-0.242830
16	6	0	1.586360	1.377007	-1.684555
17	6	0	0.914344	2.248613	0.527436
18	6	0	0.670016	2.217388	-2.263359
19	1	0	2.193409	0.714905	-2.286958
20	6	0	0.014296	3.089995	-0.083249
21	1	0	1.040362	2.231246	1.604512
22	6	0	-0.156547	3.074330	-1.485758
23	1	0	0.555145	2.225923	-3.343757
24	1	0	-0.596768	3.760121	0.514901
25	6	0	-1.143217	3.986130	-2.147720
26	1	0	-0.655327	4.929976	-2.432116
27	1	0	-1.546488	3.543504	-3.063425
28	1	0	-1.972132	4.235547	-1.479332
29	8	0	-5.112301	-1.489672	0.752105
30	6	0	-4.006291	-1.042974	0.461967
31	6	0	-3.099255	-1.701829	-0.506430
32	6	0	-3.472539	0.248090	0.937329



33	6	0	-1.955002	-1.126122	-0.991000
34	6	0	-2.316995	0.804979	0.450604
35	6	0	-1.550835	0.140504	-0.523530
36	1	0	-1.367708	-1.653842	-1.734237
37	1	0	-2.015355	1.772903	0.824965
38	1	0	-0.651691	0.582837	-0.913493
39	7	0	-3.453082	-3.031049	-0.998416
40	8	0	-3.255527	-3.255630	-2.195492
41	8	0	-3.887812	-3.834359	-0.182206
42	7	0	-4.198696	1.003580	1.953518
43	8	0	-4.855560	0.377081	2.776173
44	8	0	-4.073567	2.235415	1.932622

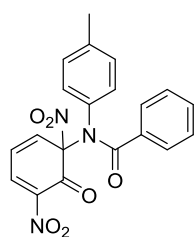


TS-C-1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.124895	-2.048780	1.432190
2	6	0	2.889908	-1.688845	1.973888
3	6	0	1.801691	-1.464839	1.133408
4	6	0	1.946607	-1.616341	-0.251839
5	6	0	3.185417	-1.985423	-0.791724
6	6	0	4.271891	-2.194573	0.049872
7	1	0	4.976720	-2.209177	2.086808
8	1	0	2.777183	-1.575772	3.048236
9	1	0	0.845650	-1.163913	1.548954
10	1	0	3.275248	-2.077279	-1.868131
11	1	0	5.237557	-2.460153	-0.369124
12	6	0	0.808135	-1.405749	-1.179389
13	8	0	0.776559	-1.797500	-2.333792
14	7	0	-0.278855	-0.663868	-0.666207
15	6	0	-1.402774	-1.289563	-0.355915
16	6	0	-1.597350	-2.717448	-0.470323
17	6	0	-2.503278	-0.502041	0.133532
18	6	0	-2.804989	-3.278986	-0.142969

19	1	0	-0.787452	-3.327314	-0.853079
20	6	0	-3.703991	-1.092898	0.451839
21	1	0	-2.368946	0.564072	0.252037
22	6	0	-3.885421	-2.485281	0.320620
23	1	0	-2.946909	-4.351616	-0.241953
24	1	0	-4.522586	-0.477887	0.813148
25	6	0	-5.201889	-3.124222	0.641779
26	1	0	-5.829730	-2.474320	1.256720
27	1	0	-5.752619	-3.337303	-0.285608
28	1	0	-5.067069	-4.081378	1.157294
29	8	0	-0.016991	2.115878	-1.802907
30	6	0	0.139570	2.197707	-0.583721
31	6	0	-0.927054	2.647356	0.326212
32	6	0	1.358784	1.819392	0.150033
33	6	0	-0.832091	2.631627	1.697864
34	6	0	1.458561	1.866336	1.531058
35	6	0	0.369886	2.247640	2.314361
36	1	0	-1.689976	2.935520	2.287940
37	1	0	2.400247	1.579431	1.981904
38	1	0	0.454295	2.261731	3.395323
39	7	0	-2.182855	3.103638	-0.250893
40	8	0	-3.226732	2.719322	0.306004
41	8	0	-2.142087	3.840109	-1.225945
42	7	0	2.544541	1.386303	-0.574867
43	8	0	2.410487	0.954683	-1.717955
44	8	0	3.628705	1.457813	0.018177

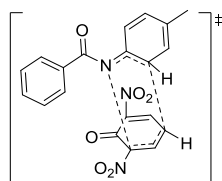
**Int-C-1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.120161	-2.861025	-0.139834
2	6	0	3.790635	-2.120476	-1.277154
3	6	0	2.476431	-1.714676	-1.491699

4	6	0	1.489147	-2.025607	-0.549830
5	6	0	1.814853	-2.788302	0.576981
6	6	0	3.129785	-3.202611	0.781109
7	1	0	5.147201	-3.173396	0.026208
8	1	0	4.558789	-1.857839	-1.998363
9	1	0	2.210222	-1.140416	-2.370923
10	1	0	1.043903	-3.046359	1.294800
11	1	0	3.378909	-3.788574	1.660773
12	6	0	0.057001	-1.676993	-0.818753
13	8	0	-0.575434	-2.193655	-1.716403
14	7	0	-0.602383	-0.818834	0.109021
15	6	0	-2.032854	-0.706641	-0.074880
16	6	0	-2.876858	-1.499165	0.700399
17	6	0	-2.567291	0.187150	-1.003854
18	6	0	-4.257650	-1.383863	0.556339
19	1	0	-2.442388	-2.192309	1.414063
20	6	0	-3.948689	0.297283	-1.136906
21	1	0	-1.902205	0.776453	-1.626445
22	6	0	-4.815208	-0.485714	-0.362909
23	1	0	-4.912917	-1.999339	1.167124
24	1	0	-4.361708	0.995430	-1.860277
25	6	0	-6.310231	-0.387713	-0.539519
26	1	0	-6.656468	-1.069275	-1.327207
27	1	0	-6.840865	-0.655234	0.379758
28	1	0	-6.614322	0.623664	-0.827915
29	8	0	0.928005	0.833114	-1.491216
30	6	0	0.704489	1.254347	-0.378573
31	6	0	0.876560	2.666471	0.019380
32	6	0	0.031163	0.330649	0.688483
33	6	0	0.105027	3.211360	0.982019
34	6	0	-0.899589	1.075439	1.614846
35	6	0	-0.822978	2.408596	1.757709
36	1	0	0.180385	4.278062	1.163787
37	1	0	-1.550084	0.465689	2.228311
38	1	0	-1.454382	2.914916	2.479973
39	7	0	1.813584	3.518960	-0.718419
40	8	0	1.642946	4.737768	-0.648685
41	8	0	2.721978	2.959908	-1.320715
42	7	0	1.190826	-0.098246	1.682055
43	8	0	2.285400	0.414326	1.500733
44	8	0	0.874391	-0.853422	2.584739

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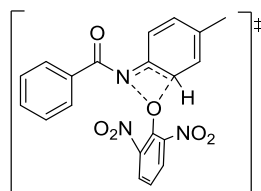


TS-C-2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.670396	-0.919485	-0.814190
2	6	0	-3.876059	0.070734	-1.394859
3	6	0	-2.513094	-0.146729	-1.567197
4	6	0	-1.938139	-1.358189	-1.155390
5	6	0	-2.743867	-2.357336	-0.589313
6	6	0	-4.104488	-2.134848	-0.416641
7	1	0	-5.731890	-0.743254	-0.665027
8	1	0	-4.310521	1.018749	-1.696312
9	1	0	-1.885062	0.614998	-2.010720
10	1	0	-2.280963	-3.287865	-0.278902
11	1	0	-4.725342	-2.900345	0.039123
12	6	0	-0.485865	-1.611604	-1.286209
13	8	0	-0.002999	-2.738816	-1.303075
14	7	0	0.271043	-0.422360	-1.438511
15	6	0	1.545855	-0.371347	-1.147356
16	6	0	2.210727	0.902153	-1.420435
17	6	0	2.361040	-1.406564	-0.530358
18	6	0	3.628586	0.984824	-1.398378
19	6	0	3.708138	-1.240505	-0.439852
20	1	0	1.881825	-2.309644	-0.184713
21	6	0	4.382177	-0.057247	-0.914697
22	1	0	4.110163	1.895194	-1.744388
23	1	0	4.311388	-2.030887	-0.000715
24	6	0	5.881579	-0.002830	-0.861167
25	1	0	6.321463	-0.811627	-1.457957
26	1	0	6.267347	0.948910	-1.235857
27	1	0	6.239562	-0.140289	0.167175
28	8	0	-1.891828	0.076383	1.586873
29	6	0	-0.853486	0.673733	1.354912
30	6	0	0.483046	0.241687	1.822473
31	6	0	-0.768120	1.880244	0.490503
32	6	0	1.648053	0.837339	1.452154
33	6	0	0.395843	2.477956	0.127513

34	6	0	1.649752	1.926607	0.524246
35	1	0	2.584630	0.449165	1.833112
36	1	0	0.361018	3.357999	-0.505463
37	7	0	0.576445	-0.912688	2.714622
38	8	0	1.564118	-1.646340	2.572928
39	8	0	-0.306596	-1.070663	3.546466
40	7	0	-2.010980	2.510013	0.040475
41	8	0	-2.955563	2.518463	0.817415
42	8	0	-2.009133	3.013810	-1.088619
43	1	0	2.532885	2.548705	0.458798
44	1	0	1.636267	1.611191	-2.004706

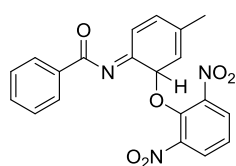


**TS-D-1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.648634	2.464511	0.270955
2	6	0	-3.125429	1.561671	-0.656422
3	6	0	-1.774426	1.606146	-0.991852
4	6	0	-0.942966	2.561320	-0.390761
5	6	0	-1.470589	3.474682	0.533135
6	6	0	-2.820078	3.423058	0.864108
7	1	0	-4.702489	2.424727	0.533117
8	1	0	-3.765025	0.819230	-1.124263
9	1	0	-1.366021	0.896903	-1.698903
10	1	0	-0.807495	4.206339	0.982283
11	1	0	-3.229121	4.125977	1.584064
12	6	0	0.506204	2.632377	-0.680423
13	8	0	1.220306	3.589229	-0.403356
14	7	0	1.024178	1.536058	-1.399140
15	6	0	2.083941	0.880304	-1.006456
16	6	0	2.833493	1.136593	0.209271
17	6	0	2.472750	-0.251724	-1.821492
18	6	0	3.891879	0.327904	0.537564
19	1	0	2.578603	2.000020	0.804702

20	6	0	3.528061	-1.047219	-1.454211
21	1	0	1.875964	-0.445117	-2.704124
22	6	0	4.251387	-0.777612	-0.269993
23	1	0	4.461589	0.525655	1.440553
24	1	0	3.806534	-1.903183	-2.061227
25	6	0	5.375111	-1.673487	0.151821
26	1	0	5.014311	-2.386627	0.907014
27	1	0	5.772941	-2.252053	-0.686177
28	1	0	6.188512	-1.105181	0.614370
29	8	0	0.145048	-0.799670	-0.649467
30	6	0	-0.704692	-1.311844	0.114392
31	6	0	-1.843687	-2.098702	-0.333856
32	6	0	-0.604920	-1.249171	1.565117
33	6	0	-2.688520	-2.768863	0.532508
34	6	0	-1.445627	-1.938520	2.426179
35	6	0	-2.501947	-2.690506	1.916716
36	1	0	-3.496490	-3.355671	0.111263
37	1	0	-1.270582	-1.864697	3.493681
38	1	0	-3.177744	-3.209246	2.587196
39	7	0	-2.119636	-2.231006	-1.759009
40	8	0	-2.677538	-3.268528	-2.133360
41	8	0	-1.806671	-1.307669	-2.511751
42	7	0	0.436361	-0.446682	2.164886
43	8	0	0.691371	0.647409	1.646082
44	8	0	0.990273	-0.867166	3.185789



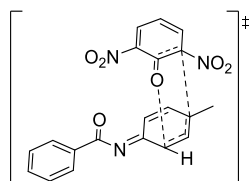
**Int-D-1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.984351	-2.157062	1.372491
2	6	0	-3.608852	-2.235510	1.147473
3	6	0	-2.996015	-1.365666	0.247728
4	6	0	-3.765174	-0.406906	-0.425792
5	6	0	-5.145519	-0.329137	-0.196358

6	6	0	-5.753036	-1.203159	0.698905
7	1	0	-5.458921	-2.838469	2.073372
8	1	0	-3.011949	-2.975199	1.672973
9	1	0	-1.928167	-1.423687	0.071347
10	1	0	-5.715891	0.424493	-0.728892
11	1	0	-6.823273	-1.143172	0.874922
12	6	0	-3.155132	0.576372	-1.365521
13	8	0	-3.792356	1.452051	-1.930249
14	7	0	-1.790872	0.373246	-1.631663
15	6	0	-0.869195	1.071417	-1.085947
16	6	0	-1.076547	2.160340	-0.134291
17	6	0	0.561685	0.678049	-1.420617
18	6	0	-0.044495	2.944135	0.235013
19	1	0	-2.080999	2.334420	0.234977
20	6	0	1.590783	1.699284	-1.075367
21	1	0	0.622420	0.373062	-2.464670
22	6	0	1.318229	2.746222	-0.273775
23	1	0	-0.206409	3.762136	0.931276
24	1	0	2.591595	1.533781	-1.462795
25	6	0	2.366645	3.732811	0.156232
26	1	0	2.078289	4.758318	-0.105174
27	1	0	2.482495	3.697514	1.247095
28	1	0	3.335679	3.518189	-0.302235
29	8	0	0.786423	-0.602881	-0.673461
30	6	0	1.865163	-0.737165	0.118918
31	6	0	3.017643	-1.409140	-0.324112
32	6	0	1.901693	-0.282047	1.449586
33	6	0	4.103483	-1.672504	0.506976
34	6	0	3.004281	-0.471712	2.277309
35	6	0	4.103062	-1.188802	1.811695
36	1	0	4.939588	-2.234580	0.108240
37	1	0	2.977605	-0.063605	3.280901
38	1	0	4.953757	-1.365873	2.460209
39	7	0	3.126502	-1.837434	-1.723837
40	8	0	3.698424	-2.903278	-1.938156
41	8	0	2.680698	-1.085840	-2.588640
42	7	0	0.752160	0.423125	2.025891
43	8	0	-0.368670	-0.017849	1.797662
44	8	0	0.998424	1.411697	2.719399

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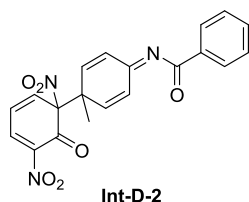
TS-D-2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.933884	1.533333	-0.397857
2	6	0	3.661211	1.405077	-0.955112
3	6	0	2.955206	0.211469	-0.813824
4	6	0	3.521801	-0.851562	-0.096517
5	6	0	4.799034	-0.715512	0.467381
6	6	0	5.504775	0.471561	0.310753
7	1	0	5.481003	2.465219	-0.510384
8	1	0	3.202258	2.235007	-1.479968
9	1	0	1.967138	0.118196	-1.253250
10	1	0	5.210243	-1.550721	1.024163
11	1	0	6.495461	0.575187	0.744110
12	6	0	2.790443	-2.121697	0.148945
13	8	0	3.184340	-2.993650	0.909565
14	7	0	1.627984	-2.330635	-0.613801
15	6	0	0.451992	-2.052800	-0.169439
16	6	0	0.175507	-1.415184	1.122977
17	6	0	-0.702695	-2.390192	-1.000414
18	6	0	-1.082553	-1.114688	1.490427
19	1	0	1.015105	-1.196783	1.774617
20	6	0	-1.964827	-2.127732	-0.602558
21	1	0	-0.493310	-2.902393	-1.933099
22	6	0	-2.248140	-1.409994	0.635003
23	1	0	-1.280605	-0.638181	2.446145
24	1	0	-2.805928	-2.429833	-1.218130
25	6	0	-3.492010	-1.848625	1.381398
26	1	0	-3.328202	-2.876388	1.727504
27	1	0	-3.675555	-1.224163	2.259158
28	1	0	-4.376825	-1.838952	0.741869
29	8	0	-0.804037	0.443466	-1.503248
30	6	0	-1.381058	0.936578	-0.546254
31	6	0	-2.734110	0.457289	-0.062531
32	6	0	-0.764980	1.943910	0.339649
33	6	0	-3.362169	1.125795	1.063210



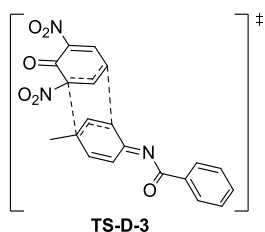
34	6	0	-1.350480	2.408444	1.472368
35	6	0	-2.674319	2.001171	1.839122
36	1	0	-4.396959	0.883950	1.266168
37	1	0	-0.813491	3.132268	2.076431
38	1	0	-3.143149	2.453982	2.705971
39	7	0	-3.720126	0.086491	-1.122239
40	8	0	-4.885139	-0.101197	-0.748913
41	8	0	-3.335355	-0.045465	-2.273842
42	7	0	0.528815	2.509176	-0.034260
43	8	0	0.733552	2.706797	-1.228986
44	8	0	1.315019	2.772366	0.877977



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.718887	1.759956	-0.261105
2	6	0	3.486603	1.529130	-0.874000
3	6	0	2.903838	0.263949	-0.813504
4	6	0	3.551690	-0.772925	-0.126607
5	6	0	4.789400	-0.533645	0.487501
6	6	0	5.372562	0.726656	0.416258
7	1	0	5.169018	2.747617	-0.308834
8	1	0	2.967395	2.332912	-1.384008
9	1	0	1.949692	0.089549	-1.300058
10	1	0	5.266944	-1.350550	1.017804
11	1	0	6.332316	0.907963	0.891872
12	6	0	2.948886	-2.128324	0.039718
13	8	0	3.446373	-2.992298	0.747072
14	7	0	1.803090	-2.394136	-0.722741
15	6	0	0.617401	-2.159789	-0.286199
16	6	0	0.316489	-1.562276	1.023969
17	6	0	-0.533205	-2.478278	-1.131455
18	6	0	-0.928073	-1.204999	1.362016
19	1	0	1.140941	-1.418587	1.715367
20	6	0	-1.781185	-2.110915	-0.810467

21	1	0	-0.320436	-3.009112	-2.053670
22	6	0	-2.134639	-1.389917	0.465412
23	1	0	-1.120564	-0.763614	2.336536
24	1	0	-2.606334	-2.343695	-1.473088
25	6	0	-3.184493	-2.219264	1.247550
26	1	0	-3.397470	-1.770603	2.222872
27	1	0	-4.113336	-2.315717	0.684706
28	1	0	-2.771429	-3.216274	1.421448
29	8	0	-1.085673	0.533070	-1.601491
30	6	0	-1.471431	0.867665	-0.502592
31	6	0	-2.655785	0.093201	0.147021
32	6	0	-0.862404	1.914508	0.340358
33	6	0	-3.258489	0.734029	1.361211
34	6	0	-1.414304	2.312619	1.508437
35	6	0	-2.648628	1.744373	2.003960
36	1	0	-4.206543	0.337692	1.710023
37	1	0	-0.924390	3.102911	2.067294
38	1	0	-3.085938	2.170887	2.900737
39	7	0	-3.788264	0.138473	-0.908635
40	8	0	-3.982865	1.242565	-1.396538
41	8	0	-4.441901	-0.868936	-1.139421
42	7	0	0.338992	2.618011	-0.119424
43	8	0	0.505816	2.723948	-1.329982
44	8	0	1.088838	3.067609	0.748073



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.938305	1.590628	1.436116
2	6	0	4.787275	2.221891	0.960216
3	6	0	3.937419	1.551092	0.083679
4	6	0	4.237001	0.242632	-0.320994
5	6	0	5.397725	-0.383721	0.154282

6	6	0	6. 243401	0. 287963	1. 030800
7	1	0	6. 599914	2. 114410	2. 120197
8	1	0	4. 556768	3. 237640	1. 267920
9	1	0	3. 052750	2. 038922	-0. 310215
10	1	0	5. 611903	-1. 394848	-0. 174830
11	1	0	7. 140434	-0. 200340	1. 399858
12	6	0	3. 342950	-0. 531911	-1. 224588
13	8	0	3. 656750	-1. 611667	-1. 706815
14	7	0	2. 123603	0. 104903	-1. 522496
15	6	0	0. 994043	-0. 511175	-1. 391826
16	6	0	0. 794042	-1. 837651	-0. 814615
17	6	0	-0. 232712	0. 228656	-1. 780032
18	6	0	-0. 438760	-2. 396080	-0. 804350
19	1	0	1. 650102	-2. 363669	-0. 412186
20	6	0	-1. 454943	-0. 491210	-1. 928057
21	1	0	-0. 051144	1. 092383	-2. 412477
22	6	0	-1. 600278	-1. 745265	-1. 391790
23	1	0	-0. 580726	-3. 372496	-0. 350951
24	1	0	-2. 305176	0. 007554	-2. 381850
25	6	0	-2. 915781	-2. 459654	-1. 390830
26	1	0	-2. 791996	-3. 533058	-1. 567222
27	1	0	-3. 405025	-2. 334185	-0. 412242
28	1	0	-3. 595639	-2. 049336	-2. 141998
29	8	0	-4. 000761	-0. 510932	0. 937269
30	6	0	-2. 981365	0. 157321	0. 835065
31	6	0	-1. 659188	-0. 239391	1. 370528
32	6	0	-2. 912703	1. 423761	0. 062089
33	6	0	-0. 495913	0. 348642	0. 990690
34	6	0	-1. 754965	1. 997786	-0. 331060
35	6	0	-0. 494875	1. 357371	-0. 031033
36	1	0	0. 439313	-0. 010178	1. 402662
37	1	0	-1. 779895	2. 880254	-0. 961745
38	1	0	0. 416275	1. 930465	-0. 167017
39	7	0	-1. 587523	-1. 333161	2. 342057
40	8	0	-0. 543819	-1. 996058	2. 364957
41	8	0	-2. 552173	-1. 510793	3. 074816
42	7	0	-4. 172279	2. 036140	-0. 365426
43	8	0	-5. 087033	2. 065348	0. 446534
44	8	0	-4. 209030	2. 493002	-1. 512082

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